

Prof. Ivano Bertini – List of Publication

1. Sabatini, A. and Bertini, I., Infrared spectra between 100 and 2500 cm⁻¹ of some complex metal cyanates, thiocyanates, and selenocyanates, **Inorg.Chem.**, 4, 959-961, 1965
2. Sabatini, A. and Bertini, I., Far-infrared spectra of oxochloro and oxobromo complexes of Nb(V), Mo(V), and W(V), **Inorg.Chem.**, 4, 204-206, 1965
3. Sabatini, A. and Bertini, I., Infrared spectra of substituted thiocyanate complexes. The effect of the substituent on bond type I, **Inorg.Chem.**, 4, 1665-1667, 1965
4. Bertini, I. and Sabatini, A., Infrared spectra of substituted thiocyanate complexes. The effect of the substituent on bond type II, **Inorg.Chem.**, 5, 1025-1028, 1966
5. Sacconi, L. and Bertini, I., Nickel(II) complexes with N,N'-tetramethylalkylenediamines, **Inorg.Nucl.Chem.Letters**, 2, 29-32, 1966
6. Sacconi, L. and Bertini, I., Complexes of copper(II) with Schiff bases formed from salicylaldehydes and N-substituted ethylenediamines, **Inorg.Chem.**, 5, 1520-1522, 1966
7. Sacconi, L. and Bertini, I., High-spin five-coordinated 3d metal complexes with pentadentate Schiff bases, **J.Am.Chem.Soc.**, 88, 5180-5185, 1966
8. Thwaites, J. D., Bertini, I., and Sacconi, L., Proton resonance studies of the solution equilibria of nickel(II) complexes with Schiff bases formed from salicylaldehydes and N,N-substituted ethylenediamines. II, **Inorg.Chem.**, 5, 1036-1041, 1966
9. Bertini, I. and Mani, F., Metal complexes of N,N,N',N'-tetramethylated diamines. II. Copper(II) and iron(II) complexes, **Inorg.Chem.**, 6, 2032-2035, 1967
10. Sacconi, L., Bertini, I., and Mani, F., Metal complexes of N,N,N',N'-tetramethyldiamines. I. Nickel(II) and cobalt(II) complexes, **Inorg.Chem.**, 6, 262-267, 1967
11. Sacconi, L., Bertini, I., and Morassi, R., High-spin five-coordinate nickel(II) and cobalt(II) complexes with a tridentate NNN Schiff base, **Inorg.Chem.**, 6, 1548-1553, 1967
12. Sacconi, L. and Bertini, I., Five-coordinate nickel(II) complexes with nitrogen-phosphorus and nitrogen-arsenic tetridentate ligands, **J.Am.Chem.Soc.**, 89, 2235-2236, 1967
13. Ciampolini, M. and Bertini, I., A ligand-field model for high-spin five-co-ordinate complexes of cobalt(II), **J.Chem.Soc.Inorg.Phys.Theor.**, 2241-2244, 1968
14. Sacconi, L., Bertini, I., and Mani, F., Five-coordination with "hybrid" ligands. II. Nickel(II) complexes with polyfunctional arsenic-containing ligands, **Inorg.Chem.**, 7, 1417-1420, 1968
15. Sacconi, L. and Bertini, I., Four- and five-coordinated complexes of cobalt(II) and nickel(II) with tridentate Schiff bases, **Inorg.Chem.**, 7, 1178-1183, 1968
16. Sacconi, L. and Bertini, I., Low- and high-spin five-coordinate cobalt(II) and nickel(II) complexes with tris(2-diphenylphosphinoethyl)amine (NP₃), **J.Am.Chem.Soc.**, 90, 5443-5446, 1968

17. Bertini, I., Johnston, D. L., and Horrocks, W. DeW., Jr., Detection of diastereoisomers in the ^1H nuclear magnetic resonance spectra of tetrahedral nickel complexes, **Chem.Commun.**, 1471-1472, 1969
18. Mani, F. and Bertini, I., Cobalt(II) and nickel(II) complexes with N,N,N'-trimethylated and triethylated alkylenediamines, **Inorg.Chim.Acta**, 3, 451-454, 1969
19. Bertini, I. and Mani, F., The existence of five-coordinate high-spin nickel(II) complexes with mixed salicylaldimine ligands, **Inorg.Chem.**, 9, 248-251, 1970
20. Bertini, I., Johnston, D. L., and Horrocks, W. DeW., Jr., High-spin five-coordinate nickel(II) complexes of a tridentate aliphatic amine containing primary amino groups, **Inorg.Chim.Acta**, 4, 79-80, 1970
21. Bertini, I., Johnston, D. L., and Horrocks, W. DeW., Jr., Synthesis and proton magnetic resonance studies of paramagnetic nickel(II) complexes containing benzaldimine groups. I. Tetrahedral complexes, **Inorg.Chem.**, 9, 693-698, 1970
22. Bertini, I., Johnston, D. L., and Horrocks, W. DeW., Jr., Synthesis and proton magnetic resonance studies of paramagnetic nickel(II) complexes containing benzaldimine groups. II. Five-coordinate complexes, **Inorg.Chem.**, 9, 698-702, 1970
23. Bertini, I., Gatteschi, D., and Wilson, L. J., A PMR investigation of the paramagnetic tris(bipyridine-N,N'-dioxide)nickel(II) and cobalt(II) complexes, **Inorg.Chim.Acta**, 629-631, 1970
24. Wilson, L. J. and Bertini, I., Cis-trans-isomerism in solution for the tris-(N-p-tolylpyridinaldimine)cobalt(II) cation, **Chem.Commun.**, 1589-1590, 1970
25. Bertini, I. and Gatteschi, D., Polarized single-crystal electronic spectrum of a high-spin Ni_3O_2 chromophore, **J.Coord.Chem.**, 1, 285-288, 1971
26. Bertini, I., Dapporto, P., Fallani, G., and Sacconi, L., A nuclear magnetic resonance study on the interconversion of the complexes $[\text{Ni}(\text{N}_3\text{P})\text{X}] \text{B}(\text{C}_6\text{H}_5)_4$ and the crystal structure of the complex $[\text{Ni}(\text{N}_3\text{P})\text{Br}] \text{B}(\text{C}_6\text{H}_5)_4$, **Inorg.Chem.**, 10, 1703-1707, 1971
27. Bertini, I. and Wilson, L. J., $\text{Ni}(\text{phen})_3^{2+}$ - $\text{Co}(\text{phen})_3^{2+}$ system: evaluation of the dipolar proton magnetic resonance shift contribution in paramagnetic cobalt(II) complexes, **J.Chem.Soc.Inorg.Phys.Theor.**, 489-492, 1971
28. Bertini, I., Ciampolini, M., and Sacconi, L., Polarized spectra of the trigonal bipyramidal CoNP_3Br chromophore, **J.Coord.Chem.**, 1, 73-74, 1971
29. Johnston, D. L., Bertini, I., and Horrocks, W. DeW., Jr., Determination of geometrical isomers in schiff bases complexes by proton magnetic resonance. Tetrahedral nickel halide complexes of ligands derived from 1,2-diaminoethane and aceto- and benzophenones, **Inorg.Chem.**, 10, 865-868, 1971
30. Wilson, L. J. and Bertini, I., NMR detection of cis and trans isomers of pseudo-octahedral metal(II) complexes with the unsymmetrical bidentate ligands N-R- pyridinaldimines, **J.Coord.Chem.**, 1, 237-242, 1971
31. Benelli, C., Bertini, I., and Gatteschi, D., Proton isotropic shifts in pseudo-tetrahedral nickel(II) and cobalt(II) complexes with salicylaldimines, **J.Chem.Soc.Dalton Trans.**, 661-663, 1972

32. Bertini, I., Gatteschi, D., and Scozzafava, A., Proton magnetic resonance spectra of six-coordinate iron(II), cobalt(II), and nickel(II) complexes with pyridine-N-oxide and benzamide, **Inorg.Chim.Acta**, 6, 185-187, 1972
33. Bertini, I. and Gatteschi, D., Single crystal polarized spectra of the Cu(en)₃SO₄ complex, **Inorg.Nucl.Chem.Letters**, 8, 207-210, 1972
34. Bertini, I., Gatteschi, D., and Mani, F., Single-crystal electronic spectra of NiPI₃ chromophore, **Inorg.Chem.**, 11, 2464-2468, 1972
35. Bertini, I., Ciampolini, M., Dapporto, P., and Gatteschi, D., Polarized single-crystal spectrum of a high-spin trigonal- bipyramidal NiN₅ chromophore, **Inorg.Chem.**, 11, 2254-2258, 1972
36. Bertini, I., Sacconi, L., and Speroni, G. P., Synthesis, characterization, and proton magnetic resonance spectra of nickel(II) and cobalt(II) complexes with o-mercaptopbenzaldimines, **Inorg.Chem.**, 11, 1323-1326, 1972
37. Bertini, I., Gatteschi, D., and Martini, G., Single-crystal polarized electronic and electron spin resonance spectra of dichlorobis(triphenylphosphine oxide)copper(II), **J.Chem.Soc.Dalton Trans.**, 1644-1646, 1973
38. Bertini, I. and Sacconi, L., Proton magnetic resonance spectra of paramagnetic molecules, **J.Mol.Struct.**, 19, 371-385, 1973
39. Bertini, I., Ciampolini, M., and Gatteschi, D., Single-crystal polarized electronic spectra of a CoN₅ chromophore, **Inorg.Chem.**, 12, 693-696, 1973
40. Bertini, I., Gatteschi, D., and Mani, F., Single-crystal polarized electronic spectra of tetra-*n*-butylammonium tribromo(quinoline)cobaltate(II), **Inorg.Chim.Acta**, 717-720, 1973
41. Bertini, I. and Gatteschi, D., Proton magnetic resonance spectra of nickel(II)- and cobalt(II)- 1,8-naphthyridine complexes. A comparison among the contact shift patterns of heterocyclic nitrogen ligands, **Inorg.Chem.**, 12, 2740-2742, 1973
42. Morassi, R., Bertini, I., and Sacconi, L., Five-coordination in iron(II), cobalt(II) and nickel(II) complexes, **Coord.Chem.Rev.**, 11, 343-402, 1973
43. Bertini, I., Gatteschi, D., and Scozzafava, A., Single crystal ESR study of the Cu(en)₃SO₄ complex, **Inorg.Chim.Acta**, 11, L17-L19, 1974
44. Bertini, I., Gatteschi, D., and Scozzafava, A., Single crystal ESR spectra of bis-*N-t*-butylpyrrol-2-aldiminocopper(II) complexes, **Gazz.Chim.Ital.**, 104, 1029-1032, 1974
45. Bertini, I., Gatteschi, D., and Scozzafava, A., Ligand field interpretation of high-spin trigonal-bipyramidal cobalt(II) complexes, **Inorg.Chem.**, 14, 812-815, 1975
46. Bertini, I., Gatteschi, D., Paoletti, P., and Scozzafava, A., A comment on the Jahn-Teller effect in the complex K₂PbCu(NO₂)₆, **Inorg.Chim.Acta**, 13, L5-L6, 1975
47. Bertini, I., Gatteschi, D., and Scozzafava, A., Single crystal polarized electronic spectra of the complex bis(*N-t*-butylpyrrole-2-carbaldimino)cobalt(II), **Inorg.Chim.Acta**, 13, 145-148, 1975

48. Bertini, I., Dapporto, P., Gatteschi, D., and Scozzafava, A., Single-crystal polarized electronic spectra of the pentakis(2- picoline N-oxide)cobalt(II) perchlorate complex, **Inorg.Chem.**, 14, 1639-1643, 1975
49. Bertini, I., Dei, A., and Scozzafava, A., Proton magnetic resonance spectra of bis(N-alkylsalicylaldiminato)copper(II) complexes, **Inorg.Chem.**, 14, 1526-1528, 1975
50. Bertini, I., Gatteschi, D., and Scozzafava, A., Single-crystal electronic spectra and ligand field parameters of some nickel(II) amine-isothiocyanato and amine-nitrito complexes, **Inorg.Chem.**, 15, 203-207, 1976
51. Bertini, I., Luchinat, C., and Scozzafava, A., ^{13}C NMR spectra of hexakis pyridine-N-oxide cobalt(II) and nickel(II) complexes, **Inorg.Chim.Acta**, 19, 201-202, 1976
52. Bertini, I., Luchinat, C., and Scozzafava, A., Interaction of cobalt bovine carbonic anhydrase with the acetate ion, **Biochim.Biophys.Acta**, 452, 239-244, 1976
53. Bertini, I., Gatteschi, D., and Scozzafava, A., Ligand field parameters, **Israel J.Chem.**, 15, 189-199, 1977
54. Bertini, I., Gatteschi, D., and Scozzafava, A., Jahn-Teller distortions of tris(ethylenediamine)copper(II) complexes, **Inorg.Chem.**, 16, 1973-1976, 1977
55. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Evidence of exchangeable protons in the donor groups of the acidic form of cobalt bovine carbonic anhydrase B, **Biochem.Biophys.Res.Commun.**, 78, 158-160, 1977
56. Bertini, I., Luchinat, C., and Scozzafava, A., Interaction of cobalt(II) bovine carbonic anhydrase with aniline, benzoate and anthranilate, **J.Am.Chem.Soc.**, 99, 581-584, 1977
57. Bertini, I., Luchinat, C., and Scozzafava, A., Interactions between a-Amino acids and cobalt(II) bovine carbonic anhydrase, **Bioinorg.Chem.**, 7, 225-231, 1977
58. Bertini, I., Luchinat, C., and Scozzafava, A., Carbon-13 longitudinal relaxation times of acetate ion in the presence of metal-substituted bovine carbonic anhydrase, **J.Chem.Soc.Dalton Trans.**, 1962-1965, 1977
59. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Proton relaxation of water solutions containing copper carbonic anhydrase, **Inorg.Chim.Acta**, 23, L15-L16, 1977
60. Bertini, I., Luchinat, C., and Scozzafava, A., Stereochemistry of cobalt(II) in cobalt bovine carbonic anhydrase and its derivatives, **Inorg.Chim.Acta**, 22, L23-L24, 1977
61. Bertini, I., Luchinat, C., and Scozzafava, A., A ^{31}P NMR study of phosphate in presence of cobalt(II)- and copper(II)- substituted bovine carbonic anhydrase B, **FEBS Lett.**, 93, 251-254, 1978
62. Bertini, I., Luchinat, C., and Scozzafava, A., Binding affinity of bicarboxylate ions for cobalt(II) bovine carbonic anhydrase, **Bioinorg.Chem.**, 9, 93-100, 1978
63. Bertini, I., Paramagnetic metal ions as structural probes for NMR investigation of inorganic and bioinorganic compounds, **J.Mol.Struct.**, 45, 173-197, 1978
64. Bertini, I., Borghi, E., and Luchinat, C., Characterization of nickel(II) bovine carbonic anhydrase and its inhibitor derivatives, **Bioinorg.Chem.**, 9, 495-504, 1978

65. Bertini, I., Dapporto, P., Gatteschi, D., and Scozzafava, A., X-ray and ESR investigation of an elongated octahedral tris-(1,2-diaminoethane) copper(II) complex, **Solid State Commun.**, 26, 749-751, 1978
66. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Characterization of cobalt(II) bovine carbonic anhydrase and of its derivatives, **J.Am.Chem.Soc.**, 100, 4873-4877, 1978
67. Bertini, I., Luchinat, C., and Scozzafava, A., Evidence of exchangeable protons in the acidic form of manganese(II) bovine carbonic anhydrase B, **FEBS Lett.**, 87, 92-94, 1978
68. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Spectroscopic investigation of copper(II) bovine carbonic anhydrase and its inhibitor derivatives, **J.Chem.Soc.Dalton Trans.**, 1269-1273, 1978
69. Barzi, D., Bertini, I., Luchinat, C., and Scozzafava, A., The electronic spectra of cobalt(II) bovine carbonic anhydrase, **Inorg.Chim.Acta**, 36, L431-L432, 1979
70. Bencini, A., Bertini, I., Gatteschi, D., and Scozzafava, A., Single-crystal ESR spectra of copper(II) complexes with geometries intermediate between a square pyramid and a trigonal bipyramidal, **Inorg.Chem.**, 17, 3194-3197, 1979
71. Bertini, I., Borghi, E., Canti, G., and Luchinat, C., Investigation of the system cobalt(II) bovine carbonic anhydrase B-trichloroacetaldehyde, **J.Inorg.Biochem.**, 11, 49-56, 1979
72. Bertini, I., Luchinat, C., and Scozzafava, A., ^{31}P NMR spectra of paramagnetic $\text{MBr}_2(\text{OPPh}_3)_2$ complexes. A breakdown in the validity of the Solomon-Bloembergen equations, **Inorg.Nucl.Chem.Letters**, 15, 89-91, 1979
73. Bertini, I., Gatteschi, D., and Scozzafava, A., Six-coordinate copper complexes with $g_{\parallel} < g_{\perp}$ in the solid state, **Coord.Chem.Rev.**, 29, 67-84, 1979
74. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Characterization of oxovanadium(IV) substituted bovine carbonic anhydrase B, **Inorg.Chim.Acta**, 36, 9-12, 1979
75. Bertini, I., Dapporto, P., Gatteschi, D., and Scozzafava, A., Static-dynamic distortions of the tris(1,2-diaminoethane)copper(II) cation $[\text{Cu}(\text{en})_3]^{2+}$. Crystal structures of the salts $[\text{Cu}(\text{en})_3]\text{[SO}_4]$ at 120 K and of $[\text{Cu}(\text{en})_3]\text{Cl}_2\cdot 0.75 \text{ en}$ at 298 K, **J.Chem.Soc.Dalton Trans.**, 1409-1414, 1979
76. Bertini, I., Borghi, E., and Luchinat, C., Investigation of the system $\text{CO}_2-\text{HCO}_3^-$ in the presence of copper(II) bovine carbonic anhydrase B, **J.Am.Chem.Soc.**, 101, 7069-7071, 1979
77. Bertini, I., Canti, G., Kozlowski, H., and Scozzafava, A., Spectroscopic characterization of copper(II) thermolysin, **J.Chem.Soc.Dalton Trans.**, 1270-1273, 1979
78. Bertini, I., Canti, G., Luchinat, C., and Mani, F., The complex cation $[\text{Co}\{\text{tris}(3,5\text{-dimethyl-1-pyrazolylmethyl)amine}\} \text{H}_2\text{O}]^{2+}$: a model for metalloenzymes containing bipositive zinc(II) chromophores with a water molecule in the coordination sphere, **Inorg.Chim.Acta**, 46, L91-L92, 1980
79. Bertini, I., Canti, G., Luchinat, C., and Romanelli, P., Cyanometallates and cobalt(II) bovine carbonic anhydrase B. Five coordination with dicyanoaurate(I), **Inorg.Chim.Acta**, 46, 211-214, 1980

80. Bertini, I., Canti, G., Grassi, R., and Scozzafava, A., Effects of planar and tetrahedral distortions on the ESR parameters of bis(salicylaldiminato)copper(II) complexes, **Inorg.Chem.**, 19, 2198-2200, 1980
81. Bertini, I., Luchinat, C., Mani, F., and Scozzafava, A., Adducts of bis(N-substituted ethylenediamine)copper(II) complexes with hexacyanoferrate(III), **Inorg.Chem.**, 19, 1333-1336, 1980
82. Bertini, I., Luchinat, C., and Scozzafava, A., The acid-base equilibria of carbonic anhydrase, **Inorg.Chim.Acta**, 46, 85-89, 1980
83. Bertini, I., Luchinat, C., and Scozzafava, A., Superoxide dismutase-thiocyanate: a study of the binding sites of anions to copper(II) in superoxide dismutase, **J.Am.Chem.Soc.**, 102, 7349-7353, 1980
84. Alberti, G., Bertini, I., Luchinat, C., and Scozzafava, A., A new class of inhibitors capable of binding both the acidic and alkaline forms of carbonic anhydrase, **Biochim.Biophys.Acta**, 668, 16-26, 1981
85. Bencini, A., Bertini, I., Canti, G., Gatteschi, D., and Luchinat, C., The EPR spectra of the inhibitor derivatives of cobalt carbonic anhydrase, **J.Inorg.Biochem.**, 14, 81-93, 1981
86. Bertini, I., Canti, G., and Luchinat, C., Water in the coordination sphere of metallocarbonic anhydrases: a solvent proton longitudinal relaxation study at several frequencies, **Inorg.Chim.Acta**, 56, 99-107, 1981
87. Bertini, I., Canti, G., and Luchinat, C., ^{17}O NMR investigation of copper(II) substituted carbonic anhydrases, **Inorg.Chim.Acta**, 56, 1-4, 1981
88. Bertini, I., Canti, G., Luchinat, C., and Mani, F., pH-dependent properties of a $\text{CoN}_4(\text{OH}_2)$ chromophore: a spectroscopic model of cobalt carbonic anhydrase, **Inorg.Chem.**, 20, 1670-1673, 1981
89. Bertini, I., Canti, G., Luchinat, C., and Mani, F., ^1H NMR spectra of the coordination sphere of cobalt- substituted carbonic anhydrase, **J.Am.Chem.Soc.**, 103, 7784-7788, 1981
90. Bertini, I., Luchinat, C., and Messori, L., A water ^{17}O NMR study of the pH dependent properties of superoxide dismutase, **Biochem.Biophys.Res.Commun.**, 101, 577-583, 1981
91. Bertini, I., The investigation of coordinated water in paramagnetic metalloproteins through nuclear magnetic resonance spectroscopy, **Comments Inorg.Chem.**, 1, 227-243, 1981
92. Bertini, I., Luchinat, C., and Borghi, E., A fourier-transform NMR investigation of $[(\text{C}_4\text{H}_9)_4\text{Z}][\text{MP}(\text{C}_6\text{H}_5)_3\text{I}_3]$ ($\text{Z} = \text{N,P}$; $\text{M} = \text{Co,Ni}$), **Inorg.Chem.**, 20, 303-306, 1981
93. Bertini, I., Borghi, E., Luchinat, C., and Scozzafava, A., 2. Binding sites of anions in superoxide dismutase, **J.Am.Chem.Soc.**, 103, 7779-7783, 1981
94. Bertini, I., Canti, G., and Luchinat, C., ^1H NMR study of cobalt(II)-substituted carboxypeptidase A, **J.Am.Chem.Soc.**, 104, 4943-4946, 1982
95. Bertini, I., Canti, G., Luchinat, C., and Messori, L., ^1H NMR detection of $\text{CoOH}_2 \leftrightarrow \text{CoOH}$ interconversions in high- spin cobalt(II) complexes, **Inorg.Chem.**, 21, 3426-3429, 1982

96. Bertini, I., Borghi, E., Luchinat, C., and Monnanni, R., Nickel carbonic anhydrase: a re-examination of the electronic spectra with the help of CD spectra, **Inorg.Chim.Acta**, 67, 99-102, 1982
97. Bertini, I., Canti, G., and Luchinat, C., Preparation and characterization of the vanadium(III) derivative of transferrin, **Inorg.Chim.Acta**, 67, L21-L23, 1982
98. Bertini, I., Luchinat, C., and Scozzafava, A., Carbonic anhydrase: an insight into the zinc binding site and into the active cavity through metal substitution, **Struct.Bonding**, 48, 45-92, 1982
99. Bertini, I., Luchinat, C., Monnanni, R., and Scozzafava, A., Different behavior of sulfonamides with respect to copper- substituted bovine and human carbonic anhydrases, **J.Inorg.Biochem.**, 16, 155-160, 1982
100. Bertini, I., Canti, G., Luchinat, C., and Borghi, E., Investigation of the system copper(II) carbonic anhydrase and $\text{HCO}_3^-/\text{CO}_2$, **J.Inorg.Biochem.**, 18, 221-229, 1983
101. Bertini, I. and Luchinat, C., Cobalt(II) as a probe of the structure and function of carbonic anhydrase, **Acc.Chem.Res.**, 16, 272-279, 1983
102. Bertini, I., Lanini, G., and Luchinat, C., Equilibrium species in cobalt(II) carbonic anhydrase, **J.Am.Chem.Soc.**, 105, 5116-5118, 1983
103. Bertini, I., Luchinat, C., Scozzafava, A., Maldotti, A., and Traverso, O., Investigation of the copper-magnesium-alkaline phosphatase system, **Inorg.Chim.Acta**, 78, 19-22, 1983
104. Bertini, I., Lanini, G., and Luchinat, C., ^1H NMR relaxation rate and coordination number in high spin cobalt(II) complexes, **Inorg.Chim.Acta**, 80, 123-126, 1983
105. Bertini, I., Luchinat, C., and Messori, L., ^{205}Tl as an NMR probe for the investigation of transferrin, **J.Am.Chem.Soc.**, 105, 1347-1350, 1983
106. Koenig, S. H., Brown III, R. D., Bertini, I., and Luchinat, C., Water exchange at the active site of carbonic anhydrase. A synthesis of the OH- and H_2O -models, **Biophys.J.**, 41, 179-187, 1983
107. Benelli, C., Bertini, I., Di Vaira, M., and Mani, F., Single-crystal X-ray and spectroscopic studies on the complex aquo[tris(3,5-dimethyl-1-pyrazolyl)methyl]amine]cobalt(II) perchlorate. A spectroscopic model of cobalt-substituted carbonic anhydrase, **Inorg.Chem.**, 23, 1422-1425, 1984
108. Bertini, I., Luchinat, C., Mancini, M., and Spina, G., The electron-nucleus dipolar coupling. The effect of zero-field splitting of an $S=3/2$ manifold, **J.Magn.Reson.**, 59, 213-222, 1984
109. Bertini, I., Luchinat, C., Monnanni, R., Scozzafava, A., and Borghi, E., Investigation of zinc-deprived bovine superoxide dismutase, **Inorg.Chim.Acta**, 91, 109-111, 1984
110. Bertini, I. and Luchinat, C., The structure of cobalt(II)-substituted carbonic anhydrase and its implications for the catalytic mechanism of the enzyme, **Ann.N.Y.Acad.Sci.**, 429, 89-98, 1984
111. Bertini, I., Lanini, G., and Luchinat, C., A water ^1H and ^{17}O N.M.R. study on PHG-modified SOD, **Inorg.Chim.Acta**, 93, 51-53, 1984

112. Bertini, I., Luchinat, C., and Monnanni, R., Carbonic anhydrase: a zinc enzyme investigated through cobalt(II) substitution: a comparison among various isoenzymes, **Rend.Acc.Lincei (Rome)**, 41-54, 1984
113. Bertini, I., Lanini, G., and Luchinat, C., Differences between high activity bovine carbonic anhydrase B and low activity human carbonic anhydrase B monitored through metal substitution, **J.Mol.Catal.**, 23, 133-144, 1984
114. Bertini, I., Gerber, M., Lanini, G., Luchinat, C., Maret, W., Rawer, S., and Zeppezauer, M., ^1H NMR investigation of the active site of cobalt(II)- substituted liver alcohol dehydrogenase, **J.Am.Chem.Soc.**, 106, 1826-1830, 1984
115. Bertini, I., Borghi, E., Luchinat, C., and Scozzafava, A., Multinuclear NMR investigation of the metal binding sites of transferrins, **J.Mol.Struct.**, 113, 191-200, 1984
116. Bertini, I., Lanini, G., and Luchinat, C., ^1H NMR spectra of reduced spinach ferredoxin, **Inorg.Chem.**, 23, 2729-2730, 1984
117. Bertini, I., Lanini, G., Luchinat, C., and Raciti, A., Are there other acidic groups capable of affecting the electronic spectra of cobalt(II) substituted carbonic anhydrase?, **Inorg.Chim.Acta**, 91, 173-177, 1984
118. Bertini, I., Luchinat, C., Messori, L., and Scozzafava, A., Cobalt(II) as an NMR probe for the investigation of the coordination sites of conalbumin, **Eur.J.Biochem.**, 141, 375-378, 1984
119. Banci, L., Bertini, I., and Luchinat, C., ^1H NMRD studies of solutions of paramagnetic metal ions in ethyleneglycol, **Inorg.Chim.Acta**, 100, 173-181, 1985
120. Banci, L., Bertini, I., and Luchinat, C., Solvent ^1H NMRD of copper(II) complexes, **Chem.Phys.Lett.**, 118, 345-347, 1985
121. Bertini, I., Luchinat, C., and Kowalewski, J., Nuclear spin relaxation in paramagnetic ($S>1/2$) systems. A comparison of two new theoretical approaches, **J.Magn.Reson.**, 62, 235-241, 1985
122. Bertini, I., Lanini, G., Luchinat, C., and Monnanni, R., Investigation of cobalt(II) substituted carboxypeptidase A interacting with azide and cyanate ions, **Inorg.Chim.Acta**, 107, 153-157, 1985
123. Bertini, I. and Luchinat, C., High spin cobalt(II) as a probe for the investigation of metalloproteins, **Adv.Inorg.Biochem.**, 6, 71-111, 1985
124. Bertini, I., Lanini, G., Luchinat, C., Mancini, M., and Spina, G., The electron-nucleus dipolar coupling in slow rotating systems. 3. The effect of isotropic exchange coupling of the electron spin with a second paramagnetic center, **J.Magn.Reson.**, 63, 56-63, 1985
125. Bertini, I., Luchinat, C., and Monnanni, R., Zinc enzymes, **J.Chem.Educ.**, 62, 924-927, 1985
126. Bertini, I., Briganti, F., Koenig, S. H., and Luchinat, C., Magnetic relaxation of solvent protons by Cu^{2+} - and VO^{2+} - substituted transferrin: theoretical analysis and biochemical implications, **Biochemistry**, 24, 6287-6290, 1985
127. Bertini, I., Dei, A., Luchinat, C., and Monnanni, R., Acid-base properties of cobalt(II)-substituted carbonic anhydrases, **Inorg.Chem.**, 24, 301-303, 1985

128. Bertini, I., Luchinat, C., and Messori, L., Spectral characterization of vanadium-transferrin systems, **J.Inorg.Biochem.**, 25, 57-60, 1985
129. Bertini, I., Briganti, F., Luchinat, C., Mancini, M., and Spina, G., The electron nucleus dipolar coupling in slow rotating systems (2): the effect of g anisotropy and hyperfine coupling when S=1/2 and I=3/2, **J.Magn.Reson.**, 63, 41-55, 1985
130. Bertini, I., Luchinat, C., and Monnanni, R., Evidence of the breaking of the copper-imidazolate bridge in copper/cobalt-substituted superoxide dismutase upon reduction of the copper(II) centers, **J.Am.Chem.Soc.**, 107, 2178-2179, 1985
131. Bertini, I., Lanini, G., Luchinat, C., Messori, L., Monnanni, R., and Scozzafava, A., Investigation of Cu₂Co₂SOD and its anion derivatives. ¹H NMR and electronic spectra, **J.Am.Chem.Soc.**, 107, 4391-4396, 1985
132. Bicknell, R., Schaeffer, A., Auld, D. S., Riordan, J. F., Monnanni, R., and Bertini, I., Protease susceptibility of zinc - and apo-carboxypeptidase A, **Biochem.Biophys.Res.Commun.**, 133, 787-793, 1985
133. Rosi, M., Sgamellotti, A., Tarantelli, F., Bertini, I., and Luchinat, C., A theoretical investigation of the copper-superoxide system. A model for the mechanism of copper-zinc superoxide dismutase, **Inorg.Chim.Acta**, 107, L21-L22, 1985
134. Banci, L., Bertini, I., Briganti, F., and Luchinat, C., The electron-nucleus dipolar coupling in slow rotating systems. 4. The effect of zero-field splitting and hyperfine coupling when S = 5/2 and I = 5/2, **J.Magn.Reson.**, 66, 58-65, 1986
135. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., Scozzafava, A., and Salvato, B., A spectroscopic investigation of Co₂Zn₂⁻ and Co₂Co₂⁻ superoxide dismutase, **Gazz.Chim.Ital.**, 116, 51-54, 1986
136. Banci, L., Bertini, I., and Luchinat, C., Electron relaxation, **Magn.Reson.Rev.**, 11, 1-40, 1986
137. Bertini, I., Luchinat, C., Messori, L., Monnanni, R., and Scozzafava, A., The metal binding properties of ovotransferrin: an investigation of cobalt(II) derivatives, **J.Biol.Chem.**, 261, 1139-1146, 1986
138. Bertini, I., Mangani, S., Messori, L., Mobilio, S., and Orioli, P. L., Exafs investigation on a N-terminal fragment of human transferrin containing a single iron binding site, **J.de Physique**, 47, 1193-1196, 1986
139. Bertini, I., Luchinat, C., Messori, L., Scozzafava, A., Pellacani, G. C., and Sola, M., ¹³C NMR study of the synergistic anion in transferrins, **Inorg.Chem.**, 25, 1782-1786, 1986
140. Owens, C., Drago, R. S., Bertini, I., Luchinat, C., and Banci, L., NMR proton relaxation in bimetallic complexes of zinc(II), nickel(II), and copper(II), **J.Am.Chem.Soc.**, 108, 3298-3303, 1986
141. Rosi, M., Sgamellotti, A., Tarantelli, F., Bertini, I., and Luchinat, C., Ab initio calculations of the Cu²⁺-O²⁻ interaction as a model for the mechanism of copper-zinc superoxide dismutase, **Inorg.Chem.**, 25, 1005-1008, 1986
142. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., and Scozzafava, A., Characterization of the cobalt(II)-substituted superoxide dismutase-phosphate system, **Inorg.Chem.**, 26, 153-156, 1987

143. Banci, L., Bertini, I., Luchinat, C., and Scozzafava, A., Nuclear relaxation in the magnetic coupled system Cu₂Co₂SOD. histidine-44 is detached upon anion binding, **J.Am.Chem.Soc.**, 109, 2328-2334, 1987
144. Banci, L., Bertini, I., Gallori, E., Luchinat, C., Paoletti, F., Polzinelli, M., and Viezzoli, M. S., A spectroscopic investigation of cobalt(II) substituted alkaline phosphatase, **J.Inorg.Biochem.**, 30, 77-85, 1987
145. Bertini, I., Luchinat, C., Owens, C., and Drago, R. S., NMR Proton Relaxation in Bimetallic Complexes Containing Co(II), **J.Am.Chem.Soc.**, 109, 5208-5212, 1987
146. Bertini, I., Viezzoli, M. S., Luchinat, C., Stafford, E., Cardin, A. D., Behnke, W. D., Bhattacharyya, L., and Brewer, C., Circular dichroism and ¹H NMR studies of Co²⁺ and Ni²⁺ substituted concanavalin A and the Lentil and Pea Lectins, **J.Biol.Chem.**, 262, 16984-16994, 1987
147. Bertini, I., Luchinat, C., Monnanni, R., Roelens, S., and Moratal Mascarell, J. M., Interaction of CO₂ and copper(II) carbonic anhydrase, **J.Am.Chem.Soc.**, 109, 7855-7856, 1987
148. Bertini, I., Lanini, G., Luchinat, C., Haas, C., Maret, W., and Zeppezauer, M., The influence of anions and inhibitors on the catalytic metal ion in Co(II)-substituted horse liver alcohol dehydrogenase, **Eur.Biophys.J.**, 14, 431-439, 1987
149. Mota De Freitas, D., Luchinat, C., Banci, L., Bertini, I., and Valentine, J. S., ³¹P NMR study of the interaction of inorganic phosphate with bovine copper-zinc superoxide dismutase, **Inorg.Chem.**, 26, 2788-2791, 1987
150. Banci, L., Bertini, I., Luchinat, C., Viezzoli, M. S., and Wang, Y., Characterization of Cu₂Co₂- and Co₂Co₂-alkaline phosphatase complexes at acidic pH, **Inorg.Chem.**, 27, 1442-1446, 1988
151. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., and Scozzafava, A., Water ¹H nuclear magnetic relaxation dispersion (NMRD) of Cu₂Zn₂ SOD with some anions and ¹H NMR spectra of Cu₂Co₂SOD in the presence of CN⁻, **Inorg.Chem.**, 27, 107-109, 1988
152. Banci, L., Bertini, I., Luchinat, C., and Hallewell, R. A., An investigation of superoxide dismutase Lys-143, Ile-143, and Glu-143 mutants: Cu₂Co₂SOD derivatives, **J.Am.Chem.Soc.**, 110, 3629-3633, 1988
153. Banci, L., Bertini, I., Luchinat, C., Viezzoli, M. S., and Wang, Y., The cobalt(II)-alkaline phosphatase system at alkaline pH, **J.Biol.Chem.**, 263, 11263-11268, 1988
154. Bertini, I., Monnanni, R., Pellacani, G. C., Sola, M., Vallee, B. L., and Auld, D. S., ¹³C NMR studies of carboxylate inhibitor binding to cobalt(II) carboxypeptidase A, **J.Inorg.Biochem.**, 32, 13-20, 1988
155. Bertini, I., Luchinat, C., and Messori, L., The role of aminoacidic residues inside the active sites of metalloproteins, **J.Pure Appl.Chem.**, 60, 1261-1261, 1988
156. Bertini, I., Hirose, J., Kozlowski, H., Luchinat, C., Messori, L., and Scozzafava, A., Effect of nonsynergistic anions on copper transferrin, **Inorg.Chem.**, 27, 1081-1086, 1988
157. Bertini, I., Luchinat, C., Messori, L., Monnanni, R., Auld, D. S., and Riordan, J. F., ¹H NMR spectroscopic characterization of binary and ternary complexes of cobalt(II) carboxypeptidase A with inhibitors, **Biochemistry**, 27, 8318-8325, 1988

158. Bertini, I., Banci, L., Brown III, R. D., Koenig, S. H., and Luchinat, C., Electronic relaxation of a copper(II) dimer in a macromolecular complex as evaluated from solvent proton relaxation, **Inorg.Chem.**, 27, 951-953, 1988
159. Bertini, I., Messori, L., Pellacani, G. C., and Sola, M., Evidence of metal-synergistic anion bond in thallium(III) transferrin, **Inorg.Chem.**, 27, 761-762, 1988
160. Bertini, I., Hayashi, T., Kuroda, Y., Luchinat, C., and Tabushi, I., ^1H NMR characterization of the system cobalt(II) bis (histamino)-B-cyclodextrin-imidazole, **Gazz.Chim.Ital.**, 118, 777-781, 1988
161. Bertini, I., Hirose, J., Luchinat, C., Messori, L., Piccioli, M., and Scozzafava, A., Kinetic studies on metal removal from transferrins by pyrophosphate, **Inorg.Chem.**, 27, 2405-2409, 1988
162. Bicknell, R., Schaeffer, A., Bertini, I., Luchinat, C., Auld, D. S., and Vallee, B. L., The interaction of anions with the active site of carboxypeptidase A, **Biochemistry**, 27, 1050-1057, 1988
163. Huettermann, J., Kappl, R., Banci, L., and Bertini, I., An ENDOR study of human and bovine erythrocyte superoxide dismutase: ^1H and ^{14}N interactions, **Biochim.Biophys.Acta**, 956, 173-188, 1988
164. Ming, L.-J., Banci, L., Luchinat, C., Bertini, I., and Valentine, J. S., NMR study of cobalt(II)-substituted yeast and human copper-zinc superoxide dismutase, **Inorg.Chem.**, 27, 728-733, 1988
165. Ming, L.-J., Banci, L., Luchinat, C., Bertini, I., and Valentine, J. S., Characterization of copper-nickel and silver-nickel bovine superoxide dismutase by ^1H NMR spectroscopy, **Inorg.Chem.**, 27, 4458-4463, 1988
166. Banci, L., Bertini, I., Luchinat, C., and Scozzafava, A., Cyanide and azide behave in a similar fashion *versus* cuprozinc superoxide dismutase, **J.Biol.Chem.**, 264, 9742-9744, 1989
167. Banci, L., Bertini, I., Luchinat, C., Piccioli, M., Scozzafava, A., and Turano, P., ^1H NOE studies on dicopper(II) dicobalt(II) superoxide dismutase, **Inorg.Chem.**, 28, 4650-4656, 1989
168. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., and Moratal Mascarell, J. M., ^1H NMR spectra of cobalt(II)-substituted carbonic anhydrase isoenzymes, **Gazz.Chim.Ital.**, 119, 23-29, 1989
169. Banci, L., Bertini, I., Luchinat, C., Scozzafava, A., and Turano, P., Binding of fluoride to copper zinc superoxide dismutase, **Inorg.Chem.**, 28, 2377-2381, 1989
170. Banci, L., Bertini, I., Hallewell, R. A., Luchinat, C., and Viezzoli, M. S., Water in the active cavity of copper/zinc superoxide dismutase. A water ^1H -nuclear-magnetic-relaxation-dispersion study, **Eur.J.Biochem.**, 184, 125-129, 1989
171. Bertini, I., Luchinat, C., Messori, L., and Vasak, M., Proton NMR studies on the cobalt(II)-metallothionein system in solution, **J.Am.Chem.Soc.**, 111, 7296-7300, 1989
172. Bertini, I., Luchinat, C., Messori, L., and Vasak, M., Proton NMR spectra of the Co_4S_{11} cluster in metallothioneins: a theoretical model, **J.Am.Chem.Soc.**, 111, 7300-7303, 1989

173. Bertini, I., Luchinat, C., Brown III, R. D., and Koenig, S. H., Relaxation of the electronic spin moment of copper(II)- macromolecular complexes in solution, **J.Am.Chem.Soc.**, 111, 3532-3536, 1989
174. Bertini, I., Luchinat, C., Viezzoli, M. S., Banci, L., Koenig, S. H., Leung, H. T., and Coleman, J. E., Copper(II) as a probe of the active centers of alkaline phosphatase, **Inorg.Chem.**, 28, 352-358, 1989
175. Bertini, I., Luchinat, C., Viezzoli, M. S., and Wang, Y., Active-site modification of SOD by H_2O_2 studied through 1H NMR of the cobalt(II)-derivative, **Arch.Biochem.Biophys.**, 269, 586-594, 1989
176. Bertini, I., Banci, L., Luchinat, C., Bielski, B. H. J., Cabelli, D., Mullenbach, G. T., and Hallewell, R. A., An investigation of a human erythrocyte SOD modified at the position 137, **J.Am.Chem.Soc.**, 111, 714-719, 1989
177. Bertini, I., Hirose, J., Messori, L., and Monnanni, R., A 1H NMR study of cobalt(II) arsanilazocarboxypeptidase A, **J.Inorg.Biochem.**, 35, 225-230, 1989
178. Schulz, C., Bertini, I., Viezzoli, M. S., Brown III, R. D., Koenig, S. H., and Coleman, J. E., Mn(II) as a probe of the active center of alkaline phosphatase, **Inorg.Chem.**, 28, 1490-1496, 1989
179. Bal, W., Bertini, I., Kozlowski, H., Monnanni, R., Scozzafava, A., and Siateki, G. Z., The unusual behavior of the inhibitor S(+) (1-amino-2- phenylethyl) phosphonic acid towards carboxypeptidase A, **J.Inorg.Biochem.**, 40, 227-235, 1990
180. Banci, L., Bencini, A., Bertini, I., Luchinat, C., and Piccioli, M., 1H NOE and ligand field studies of copper-cobalt superoxide dismutase with anions, **Inorg.Chem.**, 29, 4867-4873, 1990
181. Banci, L., Bertini, I., Luchinat, C., and Viezzoli, M. S., A comment on the 1H NMR spectra of cobalt(II) substituted superoxide dismutases with histidines deuterated in e1-position, **Inorg.Chem.**, 29, 1438-1440, 1990
182. Banci, L., Bertini, I., Cabelli, D., Hallewell, R. A., Luchinat, C., and Viezzoli, M. S., Investigation of copper-zinc superoxide dismutase Ser-137 and Ala-137 mutants, **Inorg.Chem.**, 29, 2398-2403, 1990
183. Banci, L., Bencini, A., Bertini, I., Luchinat, C., and Viezzoli, M. S., The angular overlap analysis of the spectroscopic parameters of copper zinc SOD and its mutants. Dedicated to Prof. Angelo Mangini, **Gazz.Chim.Ital.**, 120, 179-185, 1990
184. Banci, L., Bertini, I., Caliceti, P., Monsu' Scolaro, L., Schiavon, O., and Veronese, F. M., Spectroscopic characterization of polyethyleneglycol modified superoxide dismutase: 1H NMR studies on its Cu_2Co_2 derivative, **J.Inorg.Biochem.**, 39, 149-159, 1990
185. Banci, L., Bertini, I., Luchinat, C., and Piccioli, M., Transient versus steady state NOE in paramagnetic molecules. Cu_2Co_2SOD as an example, **FEBS Lett.**, 272, 175-180, 1990
186. Banci, L., Bertini, I., and Luchinat, C., The 1H NMR parameters of magnetically coupled dimers - The Fe_2S_2 proteins as an example, **Struct.Bonding**, 72, 113-135, 1990
187. Banci, L., Bertini, I., Luchinat, C., Donaire, A., Martinez, M.-J., and Moratal Mascarell, J. M., The factors governing the coordination number in the anion derivatives of carbonic anhydrase, **Comments Inorg.Chem.**, 9, 245-261, 1990

188. Barbaro, P., Bencini, A., Bertini, I., Briganti, F., and Midollini, S., The tetranuclear trianion $[\text{Fe}_4\text{Te}_4(\text{SC}_6\text{H}_5)_4]_3^-$: crystal and molecular structure and magnetic properties, **J.Am.Chem.Soc.**, 112, 7238-7246, 1990
189. Bertini, I., Luchinat, C., Rosi, M., Sgamellotti, A., and Tarantelli, F., pK_a of zinc-bound water and nucleophilicity of hydroxo- containing species. Ab initio calculations on models for zinc-enzymes, **Inorg.Chem.**, 29, 1460-1463, 1990
190. Bertini, I., Briganti, F., and Luchinat, C., Double exchange versus J-inequality in Fe_3S_4^0 clusters, **Inorg.Chim.Acta**, 175, 9-10, 1990
191. Bertini, I., Luchinat, C., Monnanni, R., Moratal Mascarell, J. M., Donaire, A., and Auld, D. S., Azide and chloride binding to carboxypeptidase A in the presence of L-phenylalanine, **J.Inorg.Biochem.**, 39, 9-16, 1990
192. Bertini, I., Briganti, F., Luchinat, C., and Scozzafava, A., ^1H NMR studies of the oxidized and partially reduced 2(4Fe-4S) ferredoxin from *Clostridium pasteurianum*, **Inorg.Chem.**, 29, 1874-1880, 1990
193. Bertini, I., Donaire, A., Messori, L., and Moratal Mascarell, J. M., Interaction of phosphate and pyrophosphate with cobalt(II) carboxypeptidase, **Inorg.Chem.**, 29, 202-205, 1990
194. Bertini, I., Banci, L., Luchinat, C., and Piccioli, M., Spectroscopic studies on $\text{Cu}_2\text{Zn}_2\text{SOD}$: a continuous advancement of investigation tools, **Coord.Chem.Rev.**, 100, 67-103, 1990
195. Bertini, I., Luchinat, C., Banci, L., and Viezzoli, M. S., ^1H NMR and relaxometry of copper-containing dimers in proteins, **Biol.Met.**, 3, 146-150, 1990
196. Bertini, I., Luchinat, C., and Vasavada, K. V., The effect of magnetic anisotropy on the longitudinal nuclear relaxation time in paramagnetic systems, **J.Magn.Reson.**, 89, 243-254, 1990
197. Bertini, I., Briganti, F., Monnanni, R., Scozzafava, A., Carlozzi, P., and Materassi, R., ^1H NMR studies of *Chromatium vinosum* cytochrome c', **Arch.Biochem.Biophys.**, 282, 84-90, 1990
198. Bertini, I., Briganti, F., and Scozzafava, A., Proton NMR spectroscopy of Flavocytochrome c_{552} from *Chromatium vinosum*, **Inorg.Chem.**, 29, 3623-3625, 1990
199. Dugad, L. B., La Mar, G. N., Banci, L., and Bertini, I., Identification of localized redox states in plant-type two-iron ferredoxins using the nuclear overhauser effect, **Biochemistry**, 29, 2263-2271, 1990
200. Banci, L., Bertini, I., Briganti, F., and Luchinat, C., The electronic structure of paramagnetic polynuclear metal clusters in proteins studied through ^1H NMR spectroscopy, **New J.Chem.**, 15, 467-477, 1991
201. Banci, L., Bertini, I., Briganti, F., Luchinat, C., Scozzafava, A., and Vicens Oliver, M., ^1H NMR spectra of oxidized high-potential iron-sulfur protein (HiPIP) from *Rhodococcus gelatinosus*. A model for oxidized HiPIPs, **Inorg.Chem.**, 30, 4517-4524, 1991
202. Banci, L., Bertini, I., and Turano, P., An investigation of Cu_2Zn_2 superoxide dismutase and its Ile-137 mutant at high pH, **Eur.Biophys.J.**, 19, 141-146, 1991

203. Banci, L., Bertini, I., Cabelli, D. E., Hallewell, R. A., Luchinat, C., and Viezzoli, M. S., Advances in understanding of the structure-function relationship in Cu,Zn superoxide dismutase, **Free Radical Res.Comms.**, 12-13, 239-251, 1991
204. Banci, L., Bertini, I., Briganti, F., Luchinat, C., Scozzafava, A., and Vicens Oliver, M., ¹H NOE studies of oxidized high potential iron sulfur protein II from *Ectothiorhodospira halophila*, **Inorg.Chim.Acta**, 180, 171-175, 1991
205. Banci, L., Bertini, I., Turano, P., Ferrer, J. C., and Mauk, A. G., Comparative ¹H NMR study of ferric low-spin cytochrome c peroxidase and horseradish peroxidase, **Inorg.Chem.**, 30, 4510-4516, 1991
206. Banci, L., Bertini, I., Turano, P., Tien, M., and Kirk, T. K., Proton NMR investigation into the basis for the relatively high redox potential of lignin peroxidase, **Proc.Natl.Acad.Sci.USA**, 88, 6956-6960, 1991
207. Banci, L., Bertini, I., Cabelli, D. E., Hallewell, R. A., Tung, J. W., and Viezzoli, M. S., A characterization of copper/zinc superoxide dismutase mutants at position 124 - Zinc-deficient proteins, **Eur.J.Biochem.**, 196, 123-128, 1991
208. Bertini, I., Capozzi, F., Luchinat, C., and Turano, P., Applications of COSY to paramagnetic heme-containing systems, **J.Magn.Reson.**, 95, 244-252, 1991
209. Bertini, I., Capozzi, F., and Luchinat, C., Water proton relaxation rate enhancements as a function of magnetic field strength and nature and size of paramagnetic solutes, **Magn.Res.Imaging**, 9, 849-853, 1991
210. Bertini, I., Capozzi, F., Luchinat, C., Piccioli, M., and Viezzoli, M. S., Assignment of active site protons in the ¹H NMR spectrum of reduced human Cu,Zn superoxide dismutase, **Eur.J.Biochem.**, 197, 691-697, 1991
211. Bertini, I., Lepori, A., Luchinat, C., and Turano, P., Role of Arg-143 in human Cu₂Zn₂SOD studied through anion binding, **Inorg.Chem.**, 30, 3363-3364, 1991
212. Bertini, I., Briganti, F., Luchinat, C., Scozzafava, A., and Sola, M., ¹H NMR spectroscopy and the electronic structure of the high potential iron-sulfur protein from *Chromatium vinosum*, **J.Am.Chem.Soc.**, 113, 1237-1245, 1991
213. Bertini, I., Luchinat, C., Piccioli, M., Vicens Oliver, M., and Viezzoli, M. S., ¹H NMR investigation of reduced copper-cobalt superoxide dismutase, **Eur.Biophys.J.**, 20, 269-279, 1991
214. Bertini, I., Briganti, F., Luchinat, C., Messori, L., Monnanni, R., Scozzafava, A., and Vallini, G., 2D ¹H NMR studies of oxidized ferredoxin from *Clostridium pasteurianum*, **FEBS Lett.**, 289, 253-256, 1991
215. Auld, D. S., Bertini, I., Donaire, A., Messori, L., and Moratal Mascarell, J. M., The pH dependent properties of cobalt(II) carboxypeptidase A inhibitor complexes, **Biochemistry**, 31, 3840-3846, 1992
216. Banci, L., Bertini, I., Carloni, P., Luchinat, C., and Orioli, P. L., Molecular dynamics simulations on HiPIP from *Chromatium vinosum* and comparison with NMR data, **J.Am.Chem.Soc.**, 114, 10683-10689, 1992

217. Banci, L., Bertini, I., Turano, P., and Vicens Oliver, M., NOE and two-dimensional correlated ¹H NMR spectroscopy of cytochrome c' from *Chromatium vinosum*, **Eur.J.Biochem.**, 204, 107-112, 1992
218. Banci, L., Bertini, I., Pease, E. A., Tien, M., and Turano, P., ¹H NMR investigation of manganese peroxidases from *Phanerochaete chrysosporium* A comparison with other peroxidases, **Biochemistry**, 31, 10009-10017, 1992
219. Banci, L., Bertini, I., Capozzi, F., and Luchinat, C., The electron-nucleus coupling: a breakthrough in the investigation of paramagnetic metalloproteins, **Int.J.Quantum Chem.**, 42, 1383-1396, 1992
220. Bertini, I., Donaire, A., Monnanni, R., Moratal Mascarell, J. M., and Salgado, J., Spectroscopic characterization of nickel(II) carboxypeptidase, **J.Chem.Soc.Dalton Trans.**, 1443-1447, 1992
221. Bertini, I., Capozzi, F., Ciurli, S., Luchinat, C., Messori, L., and Piccioli, M., Identification of the iron ions of HiPIP from *Chromatium vinosum* within the protein frame through 2D NMR experiments, **J.Am.Chem.Soc.**, 114, 3332-3340, 1992
222. Bertini, I., Capozzi, F., Luchinat, C., Piccioli, M., and Vicens Oliver, M., NMR is a unique and necessary step in the investigation of iron-sulfur proteins: the HiPIP from *R. gelatinosus* as an example, **Inorg.Chim.Acta**, 198-200, 483-491, 1992
223. Bertini, I., Luchinat, C., Ming, L.-J., Piccioli, M., Sola, M., and Valentine, J. S., Two-dimensional ¹H-NMR studies of the paramagnetic metalloenzyme copper-nickel superoxide dismutase, **Inorg.Chem.**, 31, 4433-4435, 1992
224. Bertini, I., Luchinat, C., and Xia, Z., Electron relaxation of titanium(III) hexaaqua complex detected by solvent water ¹H-NMRD spectroscopy, **Inorg.Chem.**, 31, 3152-3154, 1992
225. Bertini, I., Luchinat, C., and Xia, Z., Solvent water ¹H NMRD study of oxovanadium(IV) aquaion, **J.Magn.Reson.**, 99, 235-246, 1992
226. Bertini, I., Briganti, F., Luchinat, C., Messori, L., Monnanni, R., Scozzafava, A., and Vallini, G., ¹H NMR studies on partially and fully reduced 2(4Fe-4S) ferredoxin from *Clostridium pasteurianum*, **Eur.J.Biochem.**, 204, 831-839, 1992
227. Bertini, I., Luchinat, C., Pierattelli, R., and Vila, A. J., A multinuclear ligand NMR investigation of cyanide, cyanate and thiocyanate binding to zinc and cobalt carbonic anhydrase, **Inorg.Chem.**, 31, 3975-3979, 1992
228. Bertini, I., Messori, L., and Viezzoli, M. S., Coordination compounds and life processes, **Coord.Chem.Rev.**, 120, 163-192, 1992
229. Bertini, I., Luchinat, C., Pierattelli, R., and Vila, A. J., The interaction of acetate and formate with cobalt carbonic anhydrase. An NMR study, **Eur.J.Biochem.**, 208, 607-615, 1992
230. Banci, L., Bertini, I., Kuan, I-C., Tien, M., Turano, P., and Vila, A. J., NMR investigation of the isotopically labeled cyanide derivatives of lignin peroxidase and manganese peroxidase, **Biochemistry**, 32, 13483-13489, 1993
231. Banci, L., Bertini, I., and La Penna, G., Molecular dynamics study on carboxypeptidase A: the effect of protonation of Glu 270, **Inorg.Chem.**, 32, 2207-2211, 1993

232. Banci, L., Bertini, I., Luchinat, C., Messori, L., and Turano, P., Frontiers in 2D NMR of paramagnetic metalloproteins, **Appl.Magn.Reson.**, 4, 461-476, 1993
233. Banci, L., Bertini, I., Bini, T., Tien, M., and Turano, P., Binding of horseradish, lignin and manganese peroxidases to their respective substrate, **Biochemistry**, 32, 5825-5831, 1993
234. Banci, L., Bertini, I., Luchinat, C., and Viezzoli, M. S., pH dependent properties of SOD studied through mutants on Lys 136, **Inorg.Chem.**, 32, 1403-1406, 1993
235. Banci, L., Bertini, I., Ciurli, S., Ferretti, S., Luchinat, C., and Piccioli, M., The electronic structure of $(Fe_4S_4)^{3+}$ clusters in proteins. An investigation of the oxidized high-potential iron-sulfur protein II from *Ectothiorhodospira vacuolata*, **Biochemistry**, 32, 9387-9397, 1993
236. Banci, L., Bertini, I., Marconi, S., and Pierattelli, R., 1H NMR study of reduced heme proteins: myoglobin and cytochrome P450, **Eur.J.Biochem.**, 215, 431-437, 1993
237. Banci, L., Bertini, I., Capozzi, F., Carloni, P., Ciurli, S., Luchinat, C., and Piccioli, M., The iron-sulfur cluster in the oxidized high potential iron sulfur protein from *Ectothiorhodospira halophila*, **J.Am.Chem.Soc.**, 115, 3431-3440, 1993
238. Banci, L., Bertini, I., Eltis, L. D., and Pierattelli, R., Spectroscopic characterization of a recently isolated cytochrome P450 from *Rhodococcus rhodochrous*, **Biophys.J.**, 65, 806-813, 1993
239. Banci, L., Bertini, I., Luchinat, C., Piccioli, M., and Scozzafava, A., 1D versus 2D 1H NMR experiments in dicopper, dicobalt superoxide dismutase: a further mapping of the active site. Dedicated to Prof. Lamberto Malatesta, **Gazz.Chim.Ital.**, 123, 95-100, 1993
240. Banci, L., Bertini, I., Ferretti, S., Luchinat, C., and Piccioli, M., The structure of iron-sulfur clusters in proteins as monitored by NMR, Mössbauer, EPR and molecular dynamics, **J.Mol.Struct.**, 292, 207-220, 1993
241. Banci, L., Bertini, I., Bauer, D., Hallewell, R. A., and Viezzoli, M. S., Investigation of a new Cu,ZnSOD mutant: the Thr-Arg137 derivative, **Biochemistry**, 32, 4384-4388, 1993
242. Bencini, A., Bertini, I., and Bini, T., Angular overlap interpretation of the spectromagnetic properties of the nitrate derivative of cobalt(II) substituted carbonic anhydrase, **Inorg.Chem.**, 32, 3312-3315, 1993
243. Bertini, I., Capozzi, F., Luchinat, C., and Piccioli, M., 1H NMR investigation of oxidized and reduced HiPIP from *R. globiformis*, **Eur.J.Biochem.**, 212, 69-78, 1993
244. Bertini, I., Capozzi, F., Luchinat, C., Nicastro, G., and Xia, Z., Water proton relaxation for some lanthanide aqua ions in solution, **J.Phys.Chem.**, 101, 198-201, 1993
245. Bertini, I., Capozzi, F., Luchinat, C., and Xia, Z., Nuclear and electron relaxation of $Fe(OH_2)_6^{3+}$, **J.Phys.Chem.**, 97, 1134-1137, 1993
246. Bertini, I., Ciurli, S., Dikiy, A., and Luchinat, C., The electronic structure of the $[Fe_4Se_4]^{3+}$ clusters in *Chromatium vinosum* HiPIP and *Ectothiorhodospira halophila* HiPIP II through NMR and EPR studies, **J.Am.Chem.Soc.**, 115, 12020-12028, 1993
247. Bertini, I., Briganti, F., Calzolai, L., Messori, L., and Scozzafava, A., Selective interaction of ferricyanide with cluster I of *Clostridium pasteurianum* 2[Fe4S4] ferredoxin, **FEBS Lett.**, 332, 268-272, 1993

248. Bertini, I., Hiromi, K., Hirose, J., Sola, M., and Viezzoli, M. S., Electron transfer between copper,zinc superoxide dismutase and $\text{Fe}(\text{CN})_6^{4-}$, **Inorg.Chem.**, 32, 1106-1110, 1993
249. Bertini, I., Campos, A. P., Luchinat, C., and Teixeira, M., A Mössbauer investigation of oxidized Fe_4S_4 HiPIP II from *Ectothiorhodospira halophila*, **J.Inorg.Biochem.**, 52, 227-234, 1993
250. Bertini, I., Gaudemer, A., Luchinat, C., and Piccioli, M., Electron self-exchange in HiPIPs. A characterization of HiPIP I from *Ectothiorhodospira vacuolata*, **Biochemistry**, 32, 12887-12893, 1993
251. Bertini, I., Gori, G., Luchinat, C., and Vila, A. J., 1D and 2D NMR characterization of oxidized and reduced cytochrome c' from *Rhodococcus gelatinosus*, **Biochemistry**, 32, 776-783, 1993
252. Bertini, I., Luchinat, C., Messori, L., and Vasak, M., A two-dimensional NMR study of cobalt(II)₇ rabbit liver metallothionein, **Eur.J.Biochem.**, 211, 235-240, 1993
253. Bertini, I., Piccioli, M., Scozzafava, A., and Viezzoli, M. S., Copper, Cobalt, Superoxide Dismutase: a reexamination of the ¹H NMR spectrum through a novel selectively deuteriated derivative., **Magn.Reson.Chem.**, 31, S17-S22, 1993
254. Bertini, I., Luchinat, C., and Tarchi, D., Are true scalar proton-proton connectivities ever measured in COSY spectra of paramagnetic macromolecules?, **Chem.Phys.Lett.**, 203, 445-449, 1993
255. Bertini, I., Briganti, F., Luchinat, C., and Xia, Z., Nuclear magnetic relaxation dispersion studies of hexaaquo Mn(II) ions in water-glycerol mixtures, **J.Magn.Reson.**, 101, 198-201, 1993
256. Bertini, I., Turano, P., and Vila, A. J., NMR of paramagnetic metalloproteins, **Chem.Rev.**, 93, 2833-2932, 1993
257. Ruterjans, H. H., Messori, L., Ohlenschläger, O., Briganti, F., and Bertini, I., ¹H NMR studies on reduced high potential iron protein (HiPIP) from *Chromatium Vinosum*, **Appl.Magn.Reson.**, 4, 477-489, 1993
258. Banci, L., Bertini, I., Pierattelli, R., and Vila, A. J., ¹H ¹³C HETCOR investigations on heme-containing systems, **Inorg.Chem.**, 33, 4338-4343, 1994
259. Banci, L., Bertini, I., Eltis, L. D., Felli, I. C., Kastrau, D. H. W., Luchinat, C., Piccioli, M., Pierattelli, R., and Smith, M., The three dimensional structure in solution of the paramagnetic protein high-potential iron-sulfur protein I from *Ectothiorhodospira halophila* through nuclear magnetic resonance, **Eur.J.Biochem.**, 225, 715-725, 1994
260. Banci, L., Bertini, I., Cambria, M. T., Capozzi, F., and Dikiy, A., ¹H 1D and 2D NMR studies of the ferricytochrome c551 from *Rhodococcus gelatinosus*, **Eur.J.Biochem.**, 219, 663-669, 1994
261. Banci, L., Bertini, I., Bruni, B., Carloni, P., Luchinat, C., Mangani, S., Orioli, P. L., Piccioli, M., Rypniewski, W., and Wilson, K., X-ray structure, NMR and molecular dynamics of the reduced form of copper-zinc superoxide dismutase, **Biochem.Biophys.Res.Commun.**, 202, 1088-1095, 1994
262. Banci, L., Bertini, I., Marconi, S., Pierattelli, R., and Sligar, S. G., Cytochrome P450 and aromatic bases: a ¹H NMR study, **J.Am.Chem.Soc.**, 116, 4866-4873, 1994

263. Banci, L., Bertini, I., and La Penna, G., The enzymatic mechanism of carboxypeptidase: a molecular dynamics study, **Proteins Struct.Funct.Genet.**, 18, 186-197, 1994
264. Benelli, B., Bertini, I., Capozzi, F., and Luchinat, C., ^1H NMR studies of the CoFe_3S_4 derivative of ferredoxin from *Clostridium acidi urici*. Dedicated to Prof. Luigi Sacconi, **Gazz.Chim.Ital.**, 124, 469-474, 1994
265. Bertini, I., Dikiy, A., Luchinat, C., Piccioli, M., and Tarchi, D., NOE-NOESY, a further tool in NMR of paramagnetic metalloproteins, **J.Magn.Reson.Ser.B**, 103, 278-283, 1994
266. Bertini, I., Luchinat, C., Piccioli, M., and Tarchi, D., COSY spectra of paramagnetic macromolecules, observability, scalar effects, cross correlation effects, relaxation allowed coherence transfer, **Concepts Magn.Reson.**, 6, 307-335, 1994
267. Bertini, I., Briganti, F., Mangani, S., Nolting, H. F., and Scozzafava, A., Substrate, substrate analogue, and inhibitor interactions with the ferrous active site of catechol 2,3-dioxygenase monitored through XAS studies, **FEBS Lett.**, 350, 207-212, 1994
268. Bertini, I., Luchinat, C., Macinai, R., Piccioli, M., Scozzafava, A., and Viezzoli, M. S., Paramagnetic metal centers in proteins can be investigated through heterocorrelated NMR spectroscopy, **J.Magn.Reson.Ser.B**, B104, 95-98, 1994
269. Bertini, I., Jonsson, B.-H., Luchinat, C., Pierattelli, R., and Vila, A. J., Strategies of signal assignments in paramagnetic metalloproteins. An NMR investigation of the thiocyanate adduct of the cobalt(II)-substituted human carbonic anhydrase II, **J.Magn.Reson.Ser.B**, 104, 230-239, 1994
270. Bertini, I., Capozzi, F., Luchinat, C., Piccioli, M., and Vila, A. J., The Fe_4S_4 centers in ferredoxins studied through proton and carbon hyperfine coupling. Sequence specific assignments of cysteines in ferredoxins from *Clostridium acidi urici* and *Clostridium pasteurianum*, **J.Am.Chem.Soc.**, 116, 651-660, 1994
271. Bertini, I., Piccioli, M., Viezzoli, M. S., Chiu, C. Y., and Mullenbach, G. T., A spectroscopic characterization of a monomeric analog of copper-zinc superoxide dismutase, **Eur.J.Biophys.**, 23, 167-176, 1994
272. Bertini, I., Briganti, F., Mangani, S., Nolting, H. F., and Scozzafava, A., X-ray absorption studies on catechol 2,3 dioxygenase from *Pseudomonas putida* mt2, **Biochemistry**, 33, 10777-10784, 1994
273. Bertini, I., Luchinat, C., and Piccioli, M., Copper zinc superoxide dismutase a paramagnetic protein that provides a unique frame for the NMR investigations, **Progr.NMR Spectrosc.**, 26, 91-141, 1994
274. Bertini, I., Felli, I. C., Kastrau, D. H. W., Luchinat, C., Piccioli, M., and Viezzoli, M. S., Sequence-specific assignment of the ^1H and ^{15}N Nuclear Magnetic Resonance spectra of the reduced recombinant high potential iron sulfur protein (HiPIP) I from *Ectothiorhodospira halophila*., **Eur.J.Biochem.**, 225, 703-714, 1994
275. Bertini, I., Briganti, F., and Scozzafava, A., Aliphatic and aromatic inhibitors binding to the active site of catechol 2,3-Dioxygenase from *Pseudomonas putida* mt-2., **FEBS Lett.**, 343, 56-60, 1994

276. Zewert, T. E., Gray, H. B., and Bertini, I., Environment of the heme in myoglobins. NMRD and EPR spectroscopy of Val68X (X=Asn, Asp, and Glu). Mutants of human myoglobin., **J.Am.Chem.Soc.**, 116, 1169-1173, 1994
277. Banci, L., Bertini, I., Borsari, M., Viezzoli, M. S., and Hallewell, R. A., Mutation of the metal bridging-proton donor His 63 residue in human Cu,Zn superoxide dismutase: biochemical and biophysical analysis of the His 63 to Cys mutant, **Eur.J.Biochem.**, 232, 220-225, 1995
278. Banci, L., Bertini, I., Dikiy, A., Kastrau, D. H. W., Luchinat, C., and Sompornpisut, P., The three-dimensional solution structure of the reduced high potential iron sulfur protein *Chromatium vinosum* through NMR, **Biochemistry**, 34, 206-219, 1995
279. Banci, L., Bertini, I., Bren, K. L., Gray, H. B., Sompornpisut, P., and Turano, P., Three-dimensional solution structure of the cyanide adduct of a Met80Ala variant of *Saccharomyces cerevisiae* iso-1-cytochrome c. Identification of ligand-residue interactions in the distal heme cavity, **Biochemistry**, 34, 11385-11398, 1995
280. Banci, L., Bertini, I., Chiu, C. Y., Mullenbach, G. T., and Viezzoli, M. S., Synthesis and characterization of a monomeric mutoein of Cu/Zn superoxide dismutase with partially reconstituted enzymatic activity, **Eur.J.Biochem.**, 234, 855-860, 1995
281. Banci, L., Bertini, I., Bren, K. L., Gray, H. B., and Turano, P., pH-dependent equilibria of yeast Met80Ala-iso-1-cytochrome c probed by NMR spectroscopy: a comparison with the wild-type protein, **Chemistry and Biology**, 2, 355-363, 1995
282. Banci, L., Bertini, I., Ciurli, S., Luchinat, C., and Pierattelli, R., Rationalization of the reduction potentials within the series of the high potential iron-sulfur proteins. *Dedicated to Prof. F.Basolo*, **Inorg.Chim.Acta**, 240, 251-256, 1995
283. Banci, L., Bertini, I., Pierattelli, R., Tien, M., and Vila, A. J., Factoring of the hyperfine shifts in the cyanide adduct of lignin peroxidase from *P. chrysosporium*, **J.Am.Chem.Soc.**, 117, 8659-8667, 1995
284. Belinskii, M. I., Bertini, I., Galas, O., and Luchinat, C., The electronic structure of the $\text{Fe}_4\text{S}_4^{3+}$ cluster in proteins: the importance of double exchange parameter. Dedicated to Prof. Hitoshi Ohtaki, **Z.Naturforsch.**, 50a, 75-80, 1995
285. Bertini, I., Luchinat, C., Mangani, S., and Pierattelli, R., Carbonic anhydrase: an example of how the cavity governs the reactivity at the zinc ion, **Comments Inorg.Chem.**, 17, 1-15, 1995
286. Bertini, I., Messori, L., Golub, G., Cohen, H., and Meyerstein, D., A ^1NMR study of the complex of cobalt(II) with 2,5,8,11 tetramethyl 2,5,8,11 tetrazadodecane in aerated aqueous solutions. Dedicated to Prof. Ugo Croatto, **Inorg.Chim.Acta**, 235, 5-8, 1995
287. Bertini, I., Galas, O., Luchinat, C., and Parigi, G., A computer program for the calculation of paramagnetic enhancements of nuclear relaxation rates in slowly rotating systems, **J.Magn.Reson.Ser.A**, 113, 151-158, 1995
288. Bertini, I., Capozzi, F., Eltis, L. D., Felli, I. C., Luchinat, C., and Piccioli, M., Sequence specific assignment of ligand cysteine protons of oxidized, recombinant HiPIP I from *Ectothiorhodospira halophila*, **Inorg.Chem.**, 34, 2516-2523, 1995
289. Bertini, I. and Felli, I. C., The structure determination of proteins in solution by NMR. Now it is possible also for paramagnetic proteins, **La Chimica e l'Industria**, 9, 639-648, 1995

290. Bertini, I., Briganti, F., Mangani, S., Nolting, H. F., and Scozzafava, A., Biophysical investigation of bacterial Aromatic Extradiol Dioxygenase Involved in Biodegradation Processes, **Coord.Chem.Rev.**, 144, 321-345, 1995
291. Bertini, I., Capozzi, F., Dikiy, A., Happe, B., Luchinat, C., and Timmis, K. N., Evidence of histidine coordination to the catalytic ferrous ion in the ring-cleaving 2,2'-trihydroxybiphenyl dioxygenase from the dibenzofuran-degrading bacterium *Sphingomonas sp* strain RW1, **Biochem.Biophys.Res.Commun.**, 215, 855-860, 1995
292. Bertini, I., Dikiy, A., Kastrau, D. H. W., Luchinat, C., and Sompornpisut, P., The three dimensional solution structure of the oxidized HiPIP from *Chromatium vinosum* through NMR. Comparative analysis with the solution structure of the reduced species., **Biochemistry**, 34, 9851-9858, 1995
293. Bertini, I., Ciurli, S., and Luchinat, C., The electronic structure of FeS centers in proteins and models. A contribution to the understanding of their electron transfer properties., **Struct.Bonding**, 83, 1-54, 1995
294. Bertini, I., Eltis, L. D., Felli, I. C., Kastrau, D. H. W., Luchinat, C., and Piccioli, M., The solution structure of oxidized HiPIP I from *Ectothiorhodospira halophila*, can NMR probe rearrangements associated to electron transfer processes?, **Chemistry - A European Journal**, 1, 598-607, 1995
295. Bertini, I., Donaire, A., Feinberg, B. A., Luchinat, C., Piccioli, M., and Yuan, H., Solution structure of the oxidized 2[Fe₄S₄] ferredoxin from *Clostridium pasteurianum*, **Eur.J.Biochem.**, 232, 192-205, 1995
296. Bertini, I., Galas, O., Luchinat, C., Messori, L., and Parigi, G., A theoretical analysis of the ¹H nuclear magnetic relaxation dispersion profiles of diferric transferrin, **J.Phys.Chem.**, 99, 14217-14222, 1995
297. Bren, K. L., Gray, H. B., Banci, L., Bertini, I., and Turano, P., Paramagnetic ¹H NMR spectroscopy of the cyanide derivative of Met80Ala-iso-1-cytochrome c, **J.Am.Chem.Soc.**, 117, 8067-8073, 1995
298. Davy, S. L., Osborne, M. J., Breton, J., Moore, G. R., Thomson, A. J., Bertini, I., and Luchinat, C., Determination of the (Fe₄S₄)Cys₄ cluster geometry of *Desulfovibrio africanus* ferredoxin I by ¹H NMR spectroscopy, **FEBS Lett.**, 363, 199-204, 1995
299. Golub, G., Cohen, H., Paoletti, P., Bencini, A., Messori, L., Bertini, I., and Meyerstein, D., Use of hydrophobic ligands for the stabilization of low valent transition metal complexes. 1 effect of N-Methylation of linear tetra-aza-linear alkane ligands on the properties of their copper complexes, **J.Am.Chem.Soc.**, 117, 8353-8361, 1995
300. Turano, P., Ferrer, J. C., Cheesman, M. R., Thomson, A. J., Banci, L., Bertini, I., and Mauk, A. G., pH, electrolyte, and substrate-linked variation in active site structure of the Trp51Ala variant of cytochrome c peroxidase, **Biochemistry**, 34, 13895-13905, 1995
301. Aono, S., Bertini, I., Cowan, J. A., Luchinat, C., Rosato, A., and Viezzoli, M. S., ¹H NMR studies of the Fe₇S₈ ferredoxin from *Bacillus schlegelii*: a further attempt to understand Fe₃S₄ clusters, **J.Biol.Inorg.Chem.**, 1, 523-528, 1996
302. Babini, E., Bertini, I., Borsari, M., Capozzi, F., Dikiy, A., Eltis, L. D., and Luchinat, C., A Serine -> Cysteine Ligand Mutation in the High Potential Iron-Sulfur Protein from *Chromatium*

- vinosum* Provides Insight into the Electronic Structure of the [4Fe-4S] Cluster, **J.Am.Chem.Soc.**, 118, 75-80, 1996
303. Baistrocchi, P., Banci, L., Bertini, I., Turano, P., Bren, K. L., and Gray, H. B., Three-dimensional solution structure of *Saccharomyces cerevisiae* reduced iso-1-cytochrome *c*, **Biochemistry**, 35, 13788-13796, 1996
304. Banci, L., Bertini, I., Gori Savellini, G., and Luchinat, C., Individual Reduction Potentials of the Iron-Ions in Fe₂S₂ and high potential Fe₄S₄ ferredoxins, **Inorg.Chem.**, 35, 4248-4253, 1996
305. Banci, L., Bertini, I., Quacquarini, G., Walter, O., Diaz, A., Hervás, M., and De la Rosa, M. A., The Solution structure of cytochrome c₆ the from green alga *monoraphidium braunii*, **J.Biol.Inorg.Chem.**, 1, 330-340, 1996
306. Banci, L., Bertini, I., Bren, K. L., Cremonini, M. A., Gray, H. B., Luchinat, C., and Turano, P., The use of pseudocontact shifts to refine solution structures of paramagnetic metalloproteins: Met80Ala cyano-cytochrome *c* as an example, **J.Biol.Inorg.Chem.**, 1, 117-126, 1996
307. Banci, L., Bertini, I., Bruschi, M., Sompornpisut, P., and Turano, P., NMR characterization and solution structure determination of the oxidized cytochrome c₇ from *Desulfuromonas acetoxidans*, **Proc.Natl.Acad.Sci.USA**, 93, 14396-14400, 1996
308. Belinskii, M. I., Bertini, I., Galas, O., and Luchinat, C., An exchange coupling model for Fe4S43+ polymetallic center present in proteins and model compounds. Dedicated to Prof. H.B. Gray, **Inorg.Chim.Acta**, 243, 91-99, 1996
309. Bentrop, D., Bertini, I., Capozzi, F., Dikiy, A., Eltis, L. D., and Luchinat, C., Three dimensional structure of the reduced C77S mutant of the *Chromatium vinosum* high potential iron-sulfur protein through NMR. Comparison with the solution structure of the wild-type protein., **Biochemistry**, 35, 5928-5936, 1996
310. Bentrop, D., Bertini, I., Luchinat, C., Mendes, J., Piccioli, M., and Teixeira, M., Paramagnetic NMR of the 7Fe ferredoxin from the hyperthermoacidophilic archaeon *Desulfurolobus ambivalens* reveals structural similarity to other dicluster ferredoxins, **Eur.J.Biochem.**, 236, 92-99, 1996
311. Bertini, I., Cremonini, M. A., Ferretti, S., Lozzi, I., Luchinat, C., and Viezzoli, M. S., Arene hydroxylases: metalloenzymes catalyzing dioxygenation of aromatic compounds, **Coord.Chem.Rev.**, 151, 145-160, 1996
312. Bertini, I., Luchinat, C., and Rosato, A., The solution structure of paramagnetic metalloproteins, **Progr.Biophys.Mol.Biol.**, 66, 43-80, 1996
313. Bertini, I., Luchinat, C., Mincione, G., Parigi, G., Gassner, G. T., and Ballou, D. P., NMR studies on *Phtalate Dioxygenase*: evidence for displacement of water on binding substrate, **J.Biol.Inorg.Chem.**, 1, 468-475, 1996
314. Bertini, I., Luchinat, C., and Rosato, A., Evaluation of paramagnetic relaxation rates in a J-coupled two-spin system, **Chem.Phys.Lett.**, 250, 495-504. Erratum: (1997) 265, 677, 1996
315. Bertini, I., Felli, I. C., Luchinat, C., and Rosato, A., A Complete Relaxation Matrix Refinement of the Solution Structure of a Paramagnetic Metalloprotein: Reduced HiPIP I from *E. halophila*, **Proteins Struct.Funct.Genet.**, 24, 158-164, 1996

316. Bertini, I., Borsari, M., Bosi, M., Eltis, L. D., Felli, I. C., Luchinat, C., and Piccioli, M., The influence of a surface charge on the electronic and steric structure of a high potential iron sulfur protein, **J.Biol.Inorg.Chem.**, 1, 257-263, 1996
317. Bertini, I., Briganti, F., Luchinat, C., and Scozzafava, A., Dioxygen activation in biodegradation reactions, **New J.Chem.**, 20, 187-193, 1996
318. Bertini, I., Coutsolelos, A. G., Dikiy, A., Luchinat, C., Spyroulias, G. A., and Troganis, A., Structural Yb^{3+} and Dy^{3+} porphyrin double decker complexes. What can be obtained from ^1H NMR spectroscopy in solution through ^1H NMR, **Inorg.Chem.**, 35, 6308-6315, 1996
319. Bertini, I. and Luchinat, C., Experimental data and calculated parameters in FeS polometallic centers in proteins, **J.Biol.Inorg.Chem.**, 1, 183-185, 1996
320. Bertini, I., Couture, M. M. J., Donaire, A., Eltis, L. D., Felli, I. C., Luchinat, C., Piccioli, M., and Rosato, A., The solution structure refinement of the paramagnetic reduced HiPIP I from *Ectothiorhodospira halophila* by using stable isotope labeling and nuclear relaxation, **Eur.J.Biochem.**, 241, 440-452, 1996
321. Bertini, I., Donaire, A., Felli, I. C., Luchinat, C., and Rosato, A., From NOESY Cross-Peaks to Structural Constraints in a Paramagnetic Metalloprotein, **Magn.Reson.Chem.**, 34, 948-950, 1996
322. Bertini, I., Bren, K. L., Clemente, A., Fee, J. A., Gray, H. B., Luchinat, C., Malmström, B. G., Richards, J. H., Sanders, D., and Slutter, C. E., The Cu_a center of a soluble domain from *thermus cytochrome ba*₃: an NMR investigation of the paramagnetic protein, **J.Am.Chem.Soc.**, 46, 11658-11659, 1996
323. Lu, Y., Roe, J. A., Bender, C. J., Peisach, C. J., Banci, L., Bertini, I., Gralla, E. B., and Valentine, J., New type 2 copper-cysteinate proteins. Copper site histidine-to-cysteine mutants of yeast copper-zinc superoxide dismutase, **Inorg.Chem.**, 35, 1692-1700, 1996
324. Aono, S., Bentrop, D., Bertini, I., Luchinat, C., and Macinai, R., The D13C variant of *Bacillus schlegelii* 7Fe ferredoxin is an 8 Fe ferredoxin as revealed by ^1H -NMR spectroscopy, **FEBS Lett.**, 412, 501-505, 1997
325. Banci, L., Bertini, I., Gray, H. B., Luchinat, C., Reddig, T., Rosato, A., and Turano, P., Solution structure of oxidized horse heart cytochrome *c*, **Biochemistry**, 36, 9867-9877, 1997
326. Banci, L., Bertini, I., Bren, K. L., Gray, H. B., Sompornpisut, P., and Turano, P., Solution structure of oxidized *Saccharomyces cerevisiae* Iso-1-cytochrome *c*, **Biochemistry**, 36, 8992-9001, 1997
327. Banci, L., Bertini, I., Ferroni, F., and Rosato, A., Solution structure of reduced microsomal cytochrome *b*₅, **Eur.J.Biochem.**, 249, 270-279, 1997
328. Banci, L., Benedetto, M., Bertini, I., Del Conte, R., Piccioli, M., Richert, T., and Viezzoli, M. S., Assignment of backbone NMR resonances and secondary structural elements of a reduced monomeric mutant of copper/zinc superoxide dismutase, **Magn.Reson.Chem.**, 35, 845-853, 1997
329. Banci, L., Bertini, I., Viezzoli, M. S., Argese, E., Orsega, E., Choi Ying Chiu, and Mullenbach, G. T., Tuning the activity of Cu,Zn superoxide dismutase through site directed mutagenesis: a relatively active monomeric species, **J.Biol.Inorg.Chem.**, 2, 295-301, 1997

330. Banci, L., Bertini, I., Gori Savellini, G., Romagnoli, A., Turano, P., Cremonini, M. A., Luchinat, C., and Gray, H. B., Pseudocontact shifts as constraints for energy minimization and molecular dynamic calculations on solution structures of paramagnetic metalloproteins, **Proteins Struct.Funct.Genet.**, 29, 68-76, 1997
331. Bentrop, D., Bertini, I., Luchinat, C., Nitschke, W., and Mühlhoff, U., Characterization of the unbound 2[Fe₄S₄]-ferredoxin-like photosystem I subunit PsAC from the cyanobacterium *Synechococcus elongatus*, **Biochemistry**, 36, 13629-13637, 1997
332. Bentrop, D., Bertini, I., Cremonini, M. A., Forsén, S., Luchinat, C., and Malmendal, A., The solution structure of the paramagnetic complex of the N-terminal domain of calmodulin with two Ce³⁺ ions by ¹H NMR, **Biochemistry**, 36, 11605-11618, 1997
333. Bertini, I., Gori Savellini, G., and Luchinat, C., Are unit charges always negligible?, **J.Biol.Inorg.Chem.**, 2, 114-118, 1997
334. Bertini, I., Donaire, A., Luchinat, C., and Rosato, A., Paramagnetic relaxation as a tool for solution structure determination: *Clostridium pastorianum* ferredoxin as an example, **Proteins Struct.Funct.Genet.**, 29, 348-358, 1997
335. Bertini, I., Cowan, J. A., Luchinat, C., Natarajan, K., and Piccioli, M., Characterization of a partially unfolded high potential iron protein relevant to the folding pathway and cluster stability, **Biochemistry**, 36, 9332-9339, 1997
336. Bertini, I., Dikiy, A., Luchinat, C., Macinai, R., Viezzoli, M. S., and Vincenzini, M., An NMR study of the 7Fe-8S ferredoxin from *Rhodopseudomonas palustris* and reinterpretation of data on similar systems, **Biochemistry**, 36, 3570-3579, 1997
337. Bertini, I., Donaire, A., Felli, I. C., Luchinat, C., and Rosato, A., ¹H and ¹³C NMR studies on an oxidized HiPIP, **Inorg.Chem.**, 36, 4798-4803, 1997
338. Bertini, I., Dalvit, C., Huber, J. G., Luchinat, C., and Piccioli, M., ePHOGSY experiment on a paramagnetic protein: location of the catalytic water molecule in the heme crevice of the oxidized form of horse heart Cytochrome c, **FEBS Lett.**, 415, 45-48, 1997
339. Luchinat, C., Soriano, A., Djinovic-Carugo, K., Saraste, M., Malmström, B. G., and Bertini, I., Electronic and geometric structure of the CuA site studied by ¹H NMR in a soluble domain of cytochrome c oxidase from *paracoccus denitrificans*, **J.Am.Chem.Soc.**, 119, 11023-11027, 1997
340. Murthy, N. N., Karlin, K. D., Bertini, I., and Luchinat, C., NMR and electronic relaxation in paramagnetic Dicopper(II) compounds, **J.Am.Chem.Soc.**, 119, 2156-2162, 1997
341. Aono, S., Bentrop, D., Bertini, I., Cosenza, G., and Luchinat, C., Solution structure of an artificial Fe₈S₈ ferredoxin: the D13C variant of *Bacillus schlegelii* Fe₇S₈ ferredoxin, **Eur.J.Biochem.**, 258, 502-514, 1998
342. Aono, S., Bentrop, D., Bertini, I., Donaire, A., Luchinat, C., Niikura, Y., and Rosato, A., Solution structure of the oxidized Fe₇S₈ ferredoxin from the thermophilic bacterium *Bacillus schlegelii* by ¹H NMR spectroscopy, **Biochemistry**, 37, 9812-9826, 1998
343. Arnesano, F., Banci, L., Bertini, I., and Koulougliotis, D., Solution structure of oxidized rat microsomal cytochrome b₅ in the presence of 2 M guanidinium chloride: Monitoring the early steps in protein unfolding, **Biochemistry**, 37, 17082-17092, 1998

344. Arnesano, F., Banci, L., Bertini, I., and Felli, I. C., The solution structure of oxidized rat microsomal cytochrome b₅, **Biochemistry**, 37, 173-184, 1998
345. Assfalg, M., Banci, L., Bertini, I., Bruschi, M., and Turano, P., 800 MHz ¹H NMR solution structure refinement of oxidized cytochrome c7 from *Desulfuromonas acetoxidans*, **Eur.J.Biochem.**, 256, 261-270, 1998
346. Banci, L., Bertini, I., Luchinat, C., Pierattelli, R., Shokhirev, N. V., and Walker, F. A., Analysis of the temperature dependence of the ¹H and ¹³C isotropic shifts of horse heart ferricytochrome c: explanation of Curie and anti-Curie temperature dependence and nonlinear pseudocontact shifts in a two-level framework, **J.Am.Chem.Soc.**, 120, 8472-8479, 1998
347. Banci, L., Bertini, I., Cremonini, M. A., Gori Savellini, G., Luchinat, C., Wüthrich, K., and Güntert, P., PSEUDODYANA for NMR structure calculation of paramagnetic metalloproteins using torsion angle molecular dynamics, **J.Biomol.NMR**, 12, 553-557, 1998
348. Banci, L., Bertini, I., Reddig, T., and Turano, P., Monitoring the conformational flexibility of cytochrome c at low ionic strength by ¹H NMR spectroscopy, **Eur.J.Biochem.**, 256, 271-278, 1998
349. Banci, L., Bertini, I., Dal Pozzo, L., Del Conte, R., and Tien, M., Monitoring the role of oxalate in manganese peroxidase, **Biochemistry**, 37, 9009-9015, 1998
350. Banci, L., Bertini, I., De la Rosa, M. A., Koulougliotis, D., Navarro, J. A., and Walter, O., The solution structure of oxidized cytochrome c₆ from the green alga *Monoraphidium braunii*, **Biochemistry**, 37, 4831-4843, 1998
351. Banci, L., Benedetto, M., Bertini, I., Del Conte, R., Piccioli, M., and Viezzoli, M. S., Solution structure of reduced monomeric Q133M2 Copper, Zinc Superoxide Dismutase. Why is SOD a dimeric enzyme?, **Biochemistry**, 37, 11780-11791, 1998
352. Banci, L., Berners-Price, S., Bertini, I., Clementi, V., Luchinat, C., Spyroulias, G. A., and Turano, P., Water-protein interaction in native and partially unfolded equine cytochrome c. (Dedicated to Prof. R.R. Ernst), **Mol.Phys.**, 95, 797-808, 1998
353. Banci, L., Bertini, I., Cavazza, C., Felli, I. C., and Koulougliotis, D., Probing the backbone dynamics of oxidized and reduced rat microsomal cytochrome b₅ via ¹⁵N rotating frame NMR relaxation measurements: biological implications, **Biochemistry**, 37, 12320-12330, 1998
354. Banci, L., Bertini, I., Spyroulias, G. A., and Turano, P., The conformational flexibility of oxidized cytochrome c studied through its interaction with NH₃ and at high temperature, **Eur.J.Inorg.Chem.**, 1, 583-591, 1998
355. Banci, L., Bertini, I., Huber, J. G., Luchinat, C., and Rosato, A., Partial orientation of oxidized and reduced cytochrome b₅ at high magnetic fields: Magnetic susceptibility anisotropy contributions and consequences for protein solution structure determination, **J.Am.Chem.Soc.**, 120, 12903-12909, 1998
356. Bertini, I., Galas, O., Luchinat, C., Parigi, G., and Spina, G., Nuclear and electron relaxation in magnetic exchange coupled dimers, **J.Magn.Reson.**, 130, 33-44, 1998

357. Bertini, I., Dikiy, A., Luchinat, C., Macinai, R., and Viezzoli, M. S., ^1H NMR study of the reduced cytochrome c' from *Rhodopseudomonas palustris* containing a high spin iron(II) heme moiety, **Inorg.Chem.**, 37, 4814-4821, 1998
358. Bertini, I., Luchinat, C., Macinai, R., Martinuzzi, S., Pierattelli, R., and Viezzoli, M. S., Isolation and characterization of a cytochrome c₂ from *Rhodopseudomonas palustris*. Dedicated to Prof. W. Beck, **Inorg.Chim.Acta**, 269, 125-134, 1998
359. Bertini, I., Luchinat, C., Parigi, G., Quacquarini, G., Marzola, P., and Cavagna, F. M., Off-resonance experiments and contrast agents to improve magnetic resonance imaging, **Magn.Res.Med.**, 39, 124-131, 1998
360. Bertini, I., Felli, I. C., and Luchinat, C., High magnetic field consequences on the NMR hyperfine shifts in solution, **J.Magn.Reson.**, 134, 360-364, 1998
361. Bertini, I., Kurtz, D. M., Jr., Eidsness, M. K., Liu, G., Luchinat, C., Rosato, A., and Scott, R. A., Solution structure of reduced *Clostridium pasteurianum* rubredoxin, **J.Biol.Inorg.Chem.**, 3, 401-410, 1998
362. Bertini, I. and Piccioli, M., Nuclear Magnetic Dipole Interactions in field oriented proteins: information for Structure Determination in solution, **Chem.Tracts**, 11, 918-922, 1998
363. Bertini, I., Luchinat, C., Mincione, G., and Soriano, A., ^2H NMR Investigation of $[\text{Fe}_3\text{S}_4]^0$ cluster in 7Fe8S ferredoxin from *Bacillus schlegelii*, **Inorg.Chem.**, 37, 969-972, 1998
364. Bertini, I., Luchinat, C., Piccioli, M., and Soriano, A., Folding properties of iron sulfur proteins. (Dedicated to Prof. O. Yamauchi), **Inorg.Chim.Acta**, 283, 12-16, 1998
365. Im, S.-C., Liu, G., Luchinat, C., Sykes, A. G., and Bertini, I., The solution structure of parsley [2Fe-2S] ferredoxin, **Eur.J.Biochem.**, 258, 465-477, 1998
366. Arnesano, F., Banci, L., Bertini, I., Faraone-Mennella, J., Rosato, A., Barker, P. D., and Fersht, A. R., The solution structure of oxidized *Escherichia coli* cytochrome b₅₆₂, **Biochemistry**, 38, 8657-8670, 1999
367. Arnesano, F., Banci, L., Bertini, I., Felli, I. C., and Koulougliotis, D., Solution structure of the B form of oxidized rat microsomal cytochrome b₅ and backbone dynamics via ^{15}N rotating frame NMR relaxation measurements: Biological Implications, **Eur.J.Biochem.**, 260, 347-354, 1999
368. Assfalg, M., Banci, L., Bertini, I., Bruschi, M., Giudici-Ortoni, M. T., and Turano, P., A proton-NMR investigation of the fully reduced cytochrome c₇ from *Desulfuromonas acetoxidans*: comparison between the reduced and the oxidized forms, **Eur.J.Biochem.**, 266, 634-643, 1999
369. Babini, E., Bertini, I., Borsari, M., Capozzi, F., Luchinat, C., Di Bilio, A. J., Gray, H. B., and Ponce, A., Electron transfer in ruthenium-modified high-potential iron sulfur proteins, **J Inorg Biochem.**, 74, 266-, 1999
370. Banci, L., Bertini, I., Huber, J. G., Spyroulias, G. A., and Turano, P., Solution structure of reduced horse heart cytochrome c, **J.Biol.Inorg.Chem.**, 4, 21-31, 1999
371. Banci, L., Bertini, I., Del Conte, R., and Viezzoli, M. S., Structural and functional studies of a monomeric mutant of Cu,Zn superoxide dismutase without ARG143, **Biospectroscopy**, 5, 33-41, 1999

372. Banci, L., Bertini, I., Rosato, A., and Varani, G., Mitochondrial cytochromes *c*: a comparative analysis, **J.Biol.Inorg.Chem.**, 4, 824-837, 1999
373. Banci, L., Bertini, I., Del Conte, R., Mangani, S., Viezzoli, M. S., and Fadin, R., The solution structure of a monomeric reduced form of human Copper, Zinc Superoxide Dismutase bearing the same charge as the native protein, **J.Biol.Inorg.Chem.**, 4, 795-803, 1999
374. Banci, L., Bertini, I., Capannoli, C., Del Conte, R., and Tien, M., Spectroscopic characterization of active mutants of manganese peroxidase: mutations on the proximal side affect calcium binding on the distal side, **Biochemistry**, 38, 9617-9625, 1999
375. Bentrop, D., Bertini, I., Iacoviello, R., Luchinat, C., Niikura, Y., Piccioli, M., Presenti, C., and Rosato, A., Structural and dynamical properties of a partially unfolded Fe₄S₄ protein: the role of the cofactor in protein folding, **Biochemistry**, 38, 4669-4680, 1999
376. Bertini, I., Kowalewski, J., Luchinat, C., Nilsson, T., and Parigi, G., Nuclear spin relaxation in paramagnetic complexes of S=1: Electron spin relaxation effects, **J.Chem.Phys.**, 111, 5795-5807, 1999
377. Bertini, I., Ciurli, S., Dikiy, A., Gasanov, R., Luchinat, C., Martini, G., and Safarov, N., High-field NMR studies of oxidized blue copper proteins: the case of spinach plastocyanin, **J.Am.Chem.Soc.**, 121, 2037-2046, 1999
378. Bertini, I., Luchinat, C., Parigi, G., and Walker, F. A., Heme methyl 1H chemical shifts as structural parameters in some low spin ferriheme proteins, **J.Biol.Inorg.Chem.**, 4, 515-519, 1999
379. Bertini, I., Rosato, A., and Turano, P., Solution structure of paramagnetic metalloproteins, **Pure Appl.Chem.**, 71, 1717-1725, 1999
380. Bertini, I., Clemente, A., Rombeck, I., Rosato, A., Turano, P., Lippert, B., and Quadrifoglio, F., The three-dimensional solution structures of two DNA dodecamers through full relaxation matrix analysis, **Magn.Reson.Chem.**, 37, 564-572, 1999
381. Bertini, I. and Luchinat, C., New Applications of Paramagnetic NMR in Chemical Biology, **Curr.Opin.Chem.Biol.**, 3, 145-151, 1999
382. Dilg, A. W. E., Mincione, G., Achterhold, K., Iakovleva, O., Mentler, M., Luchinat, C., Bertini, I., and Parak, F. G., Simultaneous interpretation of Mössbauer, EPR, and 57Fe ENDOR spectra of the [Fe₄S₄] cluster in the high-potential iron protein I from *Ectothiorhodospira halophila*, **J.Biol.Inorg.Chem.**, 4, 727-741, 1999
383. Ferraroni, M., Rypniewski, W., Wilson, K. S., Viezzoli, M. S., Banci, L., Bertini, I., and Mangani, S., The crystal structure of the monomeric human SOD mutant F50/G51E/E133Q at atomic resolution. The enzyme mechanism revisited, **J.Mol.Biol.**, 288, 413-426, 1998
384. Tierney, D. L., Gassner, G. T., Luchinat, C., Bertini, I., Ballou, D. P., and Penner-Hahn, J. E., NMR characterization of substrate binding in the Phtalate Dioxygenase system, **Biochemistry**, 38, 11051-11061, 1999
385. Allegrozzi, M., Bertini, I., Janik, M. B. L., Lee, Y.-M., Liu, G., and Luchinat, C., Lanthanide induced pseudocontact shifts for solution structure refinements of macromolecules in shells up to 40 Å from the metal ion, **J.Am.Chem.Soc.**, 122, 4154-4161, 2000

386. Anelli, P. L., Bertini, I., Fragai, M., Lattuada, L., Luchinat, C., and Parigi, G., Sulfonamide-functionalised gadolinium DTPA complexes as possible contrast agents for MRI: a relaxometric investigation, **Eur.J.Inorg.Chem.**, 625-630, 2000
387. Antonkine, M. L., Bentrop, D., Bertini, I., Luchinat, C., Shen, G., Bryant, D. A., Stehlik, D., and Golbeck, J. H., Paramagnetic ^1H NMR spectroscopy of the reduced, unbond photosystem I subunit PsaC: sequence specific assignment of contact-shifted resonances and identification of mixed and equal valence Fe-Fe pairs in (4Fe-4S) centers FA- and FB-, **J.Biol.Inorg.Chem.**, 5, 381-392, 2000
388. Arnesano, F., Banci, L., Bertini, I., Ciofi-Baffoni, S., de Lumley Woodyear, T., Johnson, C. M., and Barker, P. D., Structural consequences of B - to C - type heme conversion in oxidized Escherichia Coli cytochrome b₅₆₂, **Biochemistry**, 39, 1499-1514, 2000
389. Arnesano, F., Banci, L., Bertini, I., Koulougliotis, D., and Monti, A., Monitoring mobility in the early steps of unfolding: the case of oxidized cytochrome b₅ in the presence of 2 M guanidinium chloride, **Biochemistry**, 39, 7117-7130, 2000
390. Arnesano, F., Banci, L., Bertini, I., van der Wetering, K., Czisch, M., and Kaptein, R., The auto-orientation in high magnetic field of oxidized cytochrome b₅₆₂ as source of constraints for solution structure determination, **J.Biomol.NMR**, 17, 295-304, 29-4-2000
391. Babini, E., Bertini, I., Borsari, M., Capozzi, F., Luchinat, C., Zhang, X., Moura, G. L. C., Kurnikov, I. V., Beratan, D. N., Ponce, A., Di Bilio, A. J., Winkler, J. R., and Gray, H. B., Bond-Mediated Electron Tunneling in Ruthenium-Modified High-Potential Iron-Sulfur Protein, **J.Am.Chem.Soc.**, 122, 4532-4533, 2000
392. Banci, L., Bertini, I., Rosato, A., and Scacchieri, S., Solution structure of oxidized microsomal rabbit cytochrome b₅. Factors determining the heterogeneous binding of the heme., **Eur.J.Biochem.**, 267, 755-766, 2000
393. Banci, L., Bertini, I., Cramaro, F., Del Conte, R., Rosato, A., and Viezzoli, M. S., Backbone Dynamics of Human Cu, Zn Superoxide Dismutase and of its Monomeric F50/EG51E/E133Q Mutant: The influence of Dimerization on Mobility and Function, **Biochemistry**, 39, 9108-9118, 28-4-2000
394. Bentrop, D., Bertini, I., Borsari, M., Cosenza, G., Luchinat, C., and Niikura, Y., A refined model for [Fe₃S₄]⁰ clusters in proteins, **Angew.Chem.Int.Ed.**, 39, 3620-3622, 2000
395. Bertini, I., Fragai, M., Luchinat, C., and Parigi, G., ^1H NMRD profiles of diamagnetic proteins: a model-free analysis, **Magn.Reson.Chem.**, 38, 543-550, 2000
396. Bertini, I., Castellani, F., Luchinat, C., Martini, G., Parigi, G., and Ristori, S., Partial Orientation of Cytochrome-c in a Lyotropic Liquid Crystal: Residual H-H Dipolar Coupling, **J.Phys.Chem.**, 104, 10653-10658, 2000
397. Bertini, I., Luchinat, C., Niikura, Y., and Presenti, C., Model-free analysis of a thermophilic Fe₇S₈ protein as compared to a mesophilic Fe₄S₄ protein, **Proteins Struct.Funct.Genet.**, 41, 75-85, 2000
398. Bertini, I., Luchinat, C., and Turano, P., ^{15}N chemical shift changes in cytochrome b5: redox-dependent vs. guanidinium chloride-induced changes, **J.Biol.Inorg.Chem.**, 5, 761-764, 2000

399. Bertini, I., Fernández, C. O., Karlsson, B. G., Leckner, J., Luchinat, C., Malmström, B. G., Nersessian, A. M., Pierattelli, R., Shipp, E., Valentine, J. S., and Vila, A. J., Structural information through NMR hyperfine shifts in blue copper proteins, **J.Am.Chem.Soc.**, 122, 3701-3707, 2000
400. Bertini, I., Luchinat, C., and Rosato, A., The use of propionate a-proton contact shifts as structural constraints (Dedicated to Steve Lippard), **Inorg.Chim.Acta**, 297, 199-205, 2000
401. Bertini, I., Felli, I. C., and Luchinat, C., Lanthanide induced residual dipolar couplings for the conformational investigation of peripheral 15NH₂ moieties, **J.Biomol.NMR**, 18, 347-355, 2000
402. Bertini, I., Huber, J. G., Luchinat, C., and Piccioli, M., Protein hydration and location of water molecules in oxidized horse heart cytochrome c by ¹H NMR, **J.Magn.Reson.**, 147, 1-8, 2000
403. Bertini, I., Hartmann, H. J., Klein, T., Liu, G., Luchinat, C., and Weser, U., High resolution solution structure of the protein part of Cu7 metallothionein, **Eur.J.Biochem.**, 267, 1008-1018, 2000
404. Bertini, I., Luchinat, C., and Parigi, G., The hyperfine shifts in low spin iron(III) hemes: a ligand field analysis, **Eur.J.Inorg.Chem.**, 2473-2480, 2000
405. Im, S.-C., Worrall, J. A. R., Liu, G., Aliverti, A., Zanetti, G., Luchinat, C., Bertini, I., and Sykes, A. G., Reduction of [2Fe-2S] Ferredoxins and Site of Attachment of Cr(III) using ¹H-NMR and Site-Directed Mutagenesis, **Inorg.Chem.**, 39, 1755-1764, 2000
406. Arnesano, F., Banci, L., Bertini, I., Huffman, D. L., and O'Halloran, T. V., Solution Structure of the Cu(I) and Apo forms of the Yeast Metallochaperone, Atx1, **Biochemistry**, 40, 1528-1539, 2001
407. Arnesano, F., Banci, L., Bertini, I., Cantini, F., Ciofi-Baffoni, S., Huffman, D. L., and O'Halloran, T. V., Characterization of the binding interface between the copper chaperone Atx1 and the first cytosolic domain of Ccc2 ATPase, **J.Biol.Chem.**, 276, 41365-41376, 2001
408. Assfalg, M., Banci, L., Bertini, I., Ciofi-Baffoni, S., and Barker, P. D., ¹⁵N backbone dynamics of ferricytochrome b₅₆₂: comparison with the reduced protein and R98C variant, **Biochemistry**, 40, 12761-12771, 2001
409. Banci, L., Bertini, I., Branchini, B. R., Hajieva, P., Spyroulias, G. A., and Turano, P., Dimethyl Propionate Ester Heme- Containing Cytochrome b₅: Structure and Stability, **J.Biol.Inorg.Chem.**, 6, 490-503, 2001
410. Banci, L., Bertini, I., Del Conte, R., Markey, J., and Ruiz-Dueñas, F. J., Copper trafficking: the solution structure of *Bacillus subtilis* CopZ, **Biochemistry**, 40, 15660-15668, 2001
411. Banci, L., Bertini, I., Liu, G., Reddig, T., Tang, W., Wu, Y., and Zhu, D., Effects of Extrinsic Imidazole Ligation on Molecular and Electronic Structure of Cytochrome c, **J.Biol.Inorg.Chem.**, 6, 628-637, 2001
412. Banci, L., Bertini, I., Felli, I. C., Hajieva, P., and Viezzoli, M. S., Side chain mobility as monitored by CH-CH cross correlation: the example of cytochrome b5, **J.Biomol.NMR**, 20, 1-10, 2001

413. Banci, L., Bertini, I., Ciofi-Baffoni, S., Huffman, D. L., and O'Halloran, T. V., Solution structure of the yeast copper transporter domain Ccc2a in the apo and Cu(I)-loaded states, **J.Biol.Chem.**, 276, 8415-8426, 2001
414. Barker, P. D., Bertini, I., Del Conte, R., Ferguson, S. J., Hajieva, P., Tomlinson, E. J., Turano, P., and Viezzoli, M. S., A further clue to understanding the mobility of mitochondrial yeast cytochrome c: a ¹⁵N T1p investigation of the oxidized and reduced species., **Eur.J.Biochem.**, 268, 4468-4476, 2001
415. Bertini, I., Fragai, M., Luchinat, C., and Parigi, G., Solvent ¹H NMRD Study of Hexaaquochromium(III): Inferences on Hydration and Electron Relaxation, **Inorg.Chem.**, 40, 4030-4035, 2001
416. Bertini, I., Hajieva, P., Luchinat, C., and Nerinovski, K., Redox-dependent hydration of cytochrome c and cytochrome b5 studied through ¹⁷O NMRD, **J.Am.Chem.Soc.**, 123, 12925-12926, 2001
417. Bertini, I., Kowalewski, J., Luchinat, C., and Parigi, G., Cross-correlation between the dipole-dipole interaction and the Curie spin relaxation. The effect of anisotropic magnetic susceptibility, **J.Magn.Reson.**, 152, 103-108, 2001
418. Bertini, I., Luchinat, C., and Piccioli, M., Paramagnetic Probes in Metalloproteins. Turning Limitations into Advantages, **Methods Enzymol.**, 339, 314-340, 2001
419. Bertini, I., Janik, M. B. L., Liu, G., Luchinat, C., and Rosato, A., Solution structure calculations through self-orientation in a magnetic field of cerium (III) substituted calcium-binding protein, **J.Magn.Reson.**, 148, 23-30, 2001
420. Bertini, I., Janik, M. B. L., Lee, Y.-M., Luchinat, C., and Rosato, A., Magnetic Susceptibility Tensor Anisotropies for a Lanthanide Ion Series in a Fixed Protein Matrix, **J.Am.Chem.Soc.**, 123, 4181-4188, 2001
421. Bertini, I., Lee, Y.-M., Luchinat, C., Piccioli, M., and Poggi, L., Locating the metal ion in calcium-binding proteins by using cerium(III) as a probe, **ChemBioChem**, 2, 550-558, 2001
422. Bertini, I., Donaire, A., Jiménez, B., Luchinat, C., Parigi, G., Piccioli, M., and Poggi, L., Paramagnetism-based Versus Classical Constraints: An Analysis of the Solution Structure of Ca Ln Calbindin D_{9k}, **J.Biomol.NMR**, 21, 85-98, 2001
423. Bertini, I., Ciurli, S., Dikiy, A., Fernández, C. O., Luchinat, C., Safarov, N., Shumilin, S., and Vila, A. J., The first solution structure of an oxidized paramagnetic copper (II) protein : the case of plastocyanin from the cyanobacterium *Synechocystis* PCC6803, **J.Am.Chem.Soc.**, 123, 2405-2413, 2001
424. Bertini, I., Bryant, D. A., Ciurli, S., Dikiy, A., Fernández, C. O., Luchinat, C., Safarov, N., Vila, A. J., and Zhao, J., Backbone dynamics of plastocyanin in both oxidation states. Solution structure of the reduced form and comparison with the oxidized state, **J.Biol.Chem.**, 276, 47217-47226, 2001
425. Dilg, A. W. E., Capozzi, F., Mentler, M., Iakovleva, O., Luchinat, C., Bertini, I., and Parak, F. G., Comparison and characterization of the (Fe₄S₄)^{2+/3+} centre in the wild-type and C77S mutated HiPIPs from *Chromatium vinosum* monitored by Mössbauer, ⁵⁷Fe ENDOR and EPR spectroscopies, **J.Biol.Inorg.Chem.**, 6, 232-246, 2001

426. Glaser, T., Bertini, I., Moura, J. J. G., Hedman, B., Hodgson, K. O., and Solomon, E. I., Protein Effects on the Electronic Structure of the $[\text{Fe}_4\text{S}_4]^{2+}$ Cluster in Ferredoxin and HiPIP, **J.Am.Chem.Soc.**, 123, 4859-4860, 2001
427. Hollender, D., Nerinovski, K., Kiss, T., Luchinat, C., and Bertini, I., Interaction of insulin-mimetic VO(IV) complexes with albumin and apotransferrin, **J Inorg Biochem**, 86, 267-, 2001
428. Maeyama, M., Sakane, G., Pierattelli, R., Bertini, I., and Shibahara, T., Adduct of acetylene at sulfur in an oxygen- and sulfur-bridged open cubane cluster complex of tungsten, **Inorg.Chem.**, 40, 2111-2119, 2001
429. Alhaique, F., Bertini, I., Fragai, M., Carafa, M., Luchinat, C., and 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
430. Allegrozzi, M., Bertini, I., Choi, S. N., Lee, Y.-M., and Luchinat, C., Detecting small structural changes in metalloproteins by the use of NMR pseudocontact shifts, **Eur.J.Inorg.Chem.**, 2121-2127, 2002
431. Antonkine, M. L., Liu, G., Bentrop, D., Bryant, D. A., Bertini, I., Luchinat, C., Stehlík, D., and 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, **J.Biol.Inorg.Chem.**, 7, 461-472, 2002
432. Arnesano, F., Banci, L., Bertini, I., and Thompsett, A. R., Solution structure of CopC: a cupredoxin-like protein involved in copper homeostasis., **Structure**, 10, 1337-1347, 2002
433. 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 Res.**, 12, 255-271, 2002
434. Arnesano, F. and Bertini, I., Structural genomics on metalloproteins., **Gene Function and Disease**, 3, 1337-1347, 2002
435. Arnesano, F., Banci, L., Barker, P. D., Bertini, I., Rosato, A., Su, X. C., and Viezzoli, M. S., Solution structure and characterization of the heme chaperone CcmE, **Biochemistry**, 41, 13587-13594, 2002
436. Assfalg, M., Bertini, I., Bruschi, M., Michel, C., 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 c_7 , **Proc.Natl.Acad.Sci.USA**, 99, 9750-9754, 2002
437. Assfalg, M., Bertini, I., Turano, P., Bruschi, M., Durand, M. C., Giudici-Orticoni, M. T., and Dolla, A., A quick solution structure determination of the fully oxidized double mutant K9-10A cytochrome c_7 from *Desulfuromonas acetoxidans* and mechanistic implications, **J.Biomol.NMR**, 22, 107-122, 2002
438. Banci, L., Bertini, I., Cavallaro, G., and Luchinat, C., 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, **J.Biol.Inorg.Chem.**, 7, 416-426, 2002
439. Banci, L., Bertini, I., Cantini, F., D'Onofrio, M., and Viezzoli, M. S., Structure and dynamics of copper-free SOD: The protein before binding copper, **Protein Sci.**, 11, 2479-2492, 2002

440. Banci, L., Bertini, I., Ciurli, S., Dikiy, A., Dittmer, J., Rosato, A., Sciara, G., and Thompsett, A., NMR solution structure, backbone mobility and homology modeling of c-type cytochromes from gram-positive bacteria, **ChemBioChem**, 3, 299-310, 2002
441. Banci, L., Bertini, I., Ciofi-Baffoni, S., Finney, L. A., Outten, C. E., and O'Halloran, T. V., A new zinc-protein coordination site in an intracellular metal trafficking: solution structure of the apo and Zn(II) forms of ZntA(46-118), **J.Mol.Biol.**, 323, 883-897, 2002 (IF 5.359).
442. Banci, L., Bertini, I., Ciofi-Baffoni, S., D'Onofrio, M., Gonnelli, L., Marhuenda-Egea, F. C., and 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
443. Banci, L., Bertini, I., Cramaro, F., Del Conte, R., and Viezzoli, M. S., The solution structure of reduced dimeric copper zinc SOD: the structural effects of dimerization, **Eur J.Biochem**, 269, 1905-1915, 2002
444. Barbieri, R., Bertini, I., Lee, Y.-M., Luchinat, C., and Velders A.H., Structure-independent cross-validation of residual dipolar couplings originating from internal and external orienting media, **J.Biomol.NMR**, 22, 365-368, 2002
445. Barbieri, R., Bertini, I., Cavallaro, G., Lee, Y.-M., Luchinat, C., and Rosato, A., Paramagnetically induced residual dipolar couplings for solution structure determination of lanthanide-binding proteins, **J.Am.Chem.Soc.**, 124, 5581-5587, 2002
446. Bartalesi, I., Bertini, I., Hajieva, P., Rosato, A., and Vasos, P. R., Solution structure of a mono-heme ferrocyanochrome *c* from *Shewanella putrefaciens* and structural analysis of sequence-similar proteins: functional implications., **Biochemistry**, 41, 5112-5119, 2002
447. Bartalesi, I., Bertini, I., Ghosh, K., Rosato, A., and Turano, P., The unfolding of oxidized c-type cytochromes: the instructive case of *B. pasteurii*, **J.Mol.Biol.**, 321, 693-701, 2002 (IF 5.359).
448. Bertini, I., Carrano, C. J., Luchinat, C., Piccioli, M., and Poggi, L., A ¹⁵N NMR mobility study on the Di-calcium P43M calbindin D9K and its mono La ³⁺ substituted form, **Biochemistry**, 41, 5104-5111, 2002
449. Bertini, I., Longinetti, M., Luchinat, C., Parigi, G., and Sgheri, L., Efficiency of paramagnetism-based constraints to determine the spatial arrangement of a-helical secondary structure elements, **J.Biomol.NMR**, 22, 123-136, 2002
450. Bertini, I., Luchinat, C., Provenzani, A., Rosato, A., and Vasos, P. R., Browsing gene banks for Fe₂S₂ ferredoxins and structural modeling of 87 plant-type sequences: an analysis of fold and function, **Proteins Struct.Funct.Genet.**, 46, 110-127, 2002
451. Bertini, I., Luchinat, C., and Parigi, G., Magnetic susceptibility in paramagnetic NMR, **Progr.NMR Spectrosc.**, 40, 249-273, 2002
452. Bertini, I., Dilg, A. W. E., Iakovleva, O., Luchinat, C., Mincione, G., and Parak, F., Simultaneous interpretation of Mössbauer, EPR and 57Fe ENDOR spectra of the [Fe4S4] cluster in the high-potential iron protein I Ectothiorhodospira halophila, **J.Biol.Inorg.Chem.**, 4, 727-741, 2002

453. Bertini, I., Luchinat, C., and Parigi, G., Paramagnetic constraints: an aid for quick solution structure determination of paramagnetic metalloproteins, **Concepts Magn.Reson.**, 14, 259-286, 2002
454. Bertini, I., Cavallaro, G., Cosenza, M., Kümmerle, R., Luchinat, C., Piccioli, M., and Poggi, L., Cross Correlation Rates Between Curie Spin and Dipole-Dipole relaxation in Paramagnetic Proteins: the Case of Cerium Substituted Calbindin D_{9k}, **J.Biomol.NMR**, 23, 115-125, 2002
455. Dilg, A. W. E., Grantner, K., Iakovleva, O., Parak, F., Babini, E., Bertini, I., Capozzi, F., Luchinat, C., and Meyer-Klaucke, W., Dynamics of wild type HiPIP's a Cys77Ser-mutant and a partially unfolded HiPIP, **J.Biol.Inorg.Chem.**, 7, 691-703, 2002
456. Arnesano, F., Banci, L., Bertini, I., Felli, I. C., Luchinat, C., and Thompsett, A. R., 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 (IF 6.201).
457. Arnesano, F., Banci, L., Bertini, I., Mangani, S., and Thompsett, A. R., A redox switch in CopC: an intriguing copper trafficking protein which binds copper(I) and copper(II) at different sites., **Proc.Natl.Acad.Sci.USA**, 100, 3814-3819, 2003 (IF 10.700).
458. Arnesano, F., Banci, L., Benvenuti, M., Bertini, I., Calderone, V., Mangani, S., and Viezzoli, M. S., The evolutionarily conserved trimeric structure of CutA1 proteins suggests a role in signal transduction, **J.Biol.Chem.**, 278, 45999-46006, 2003 (IF 6.70).
459. Assfalg, M., Bertini, I., Turano, P., Mauk, A. G., Winkler, J. R., and Gray, B. H., ¹⁵N-¹H residual dipolar coupling analysis of native and alkaline-K79A *S. cerevisiae* cytochrome c. **Biophys.J.**, 84, 3917-3923, 2003 (IF 4.643).
460. Assfalg, M., Bertini, I., Dolfi, A., Turano, P., Mauk, A. G., Rosell, F. I., and Gray, H. B., Structural model for an alkaline form of ferricytochrome c., **J.Am.Chem.Soc.**, 125, 2913-2922, 2003 (IF 6.201).
461. Assfalg, M., Banci, L., Bertini, I., Turano, P., and Vasos, P. R., Superoxide dismutase folding/unfolding pathway: role of the metal ions in modulating structural and dynamical features., **J.Mol.Biol.**, 330, 145-158, 2003 (IF 5.359).
462. Balatri, E., Banci, L., Bertini, I., Cantini, F., and Ciofi-Baffoni, S., Solution structure of Sco1: a thioredoxin-like protein involved in cytochrome c oxidase assembly., **Structure**, 11, 1431-1443, 2003 (IF 6.030).
463. Banci, L., Bertini, I., Ciofi-Baffoni, S., Del Conte, R., and Gonnelli, L., 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 (IF 4.064).
464. Banci, L., Bertini, I., Ciofi-Baffoni, S., Gonnelli, L., and Su, X. C., A core mutation affecting the folding properties of a soluble domain of the ATPase protein CopA from *Bacillus Subtilis*. **J.Mol.Biol.**, 331, 473-484, 2003 (IF 5.359).
465. Banci, L., Bertini, I., Felli, I. C., Krippahl, L., Kubicek, K., Moura, J. J. G., and Rosato, A., A further investigation of the cytochrome b₅ - cytochrome c complex., **J.Biol.Inorg.Chem.**, 8, 777-786, 2003 (IF 3.911).

466. Banci, L., Bertini, I., Cramaro, F., Del Conte, R., and Viezzoli, M. S., Solution structure of Apo Cu,Zn superoxide dismutase: role of metal ions in protein folding, **Biochemistry**, 42, 9543-9553, 19-8-2003
467. Banci, L., Bertini, I., Del Conte, R., Mangani, S., and Meyer-Klaucke, W., X-ray absorption spectroscopy study of CopZ, a copper chaperone in *Bacillus subtilis*. The coordination properties of the copper ion., **Biochemistry**, 8, 2467-2474, 2003 (IF 4.064).
468. Banci, L., Bertini, I., and Del Conte, R., The solution structure of apo CopZ from *Bacillus subtilis*: a further analysis of the changes associated with the presence of copper., **Biochemistry**, 42, 13422-13428, 2003 (IF 4.064).
469. Banci, L., Bertini, I., Ciofi-Baffoni, S., Gonnelli, L., and Su, X. C., Structural basis for the function of the N terminal domain of the ATPase CopA from *Bacillus subtilis*, **J.Biol.Chem.**, 278, 50506-50513, 2003 (IF 6.70).
470. Banci, L., Bertini, I., Ciulli, A., Fragai, M., Luchinat, C., and Terni, B., 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 (IF 1.729).
471. Bartalesi, I., Bertini, I., and Rosato, A., Structure and dynamics of reduced *Bacillus pasteurii* cytochrome c: oxidation state dependent properties and implications for electron transfer processes., **Biochemistry**, 42, 739-745, 2003 (IF 4.064).
472. Bermel, W., Bertini, I., Felli, I. C., Kümmel, R., and Pierattelli, R., ¹³C direct detection experiments on the paramagnetic oxidized monomeric copper, zinc superoxide dismutase, **J.Am.Chem.Soc.**, 125, 16423-16429, 2003
473. Bertini, I., Gelis, I., Katsaros, N., Luchinat, C., and Provenzani, A., Tuning the Affinity for Lanthanides of Calcium Binding Proteins., **Biochemistry**, 42, 8011-8021, 2003 (IF 4.064).
474. Bertini, I., Ghosh, K., Rosato, A., and Vasos, P. R., A high-resolution NMR study of long-lived water molecules in both oxidation states of a minimal cytochrome c., **Biochemistry**, 42, 3457-3463, 2003 (IF 4.064).
475. Bertini, I., Structural genomics., **Acc.Chem.Res.**, 36, 155-, 2003 (IF 15.901).
476. Bertini, I., Calderone, V., Fragai, M., Luchinat, C., Mangani, S., and Terni, B., X-ray structures of ternary enzyme-product-inhibitor complexes of MMP., **Angew.Chem.Int.Ed.**, 42, 2673-2676, 2003 (IF 7.671).
477. Bertini, I., Cavallaro, G., Luchinat, C., and Poli, I., A use of ramachandran potentials in protein solution structure determinations, **J.Biomol.NMR**, 4, 355-366, 2003
478. Bertini, I., Cowan, J. A., Del Bianco, C., Luchinat, C., and Mansy, S. S., Thermotoga maritima IscU. Structural characterization and dynamics of a new class of metallochaperone., **J.Mol.Biol.**, 331, 907-924, 2003 (IF 5.359).
479. Bertini, I., Luchinat, C., and Sola, M., Zinc enzymes/models, **Encyclopaedia of Chemistry**, DOI: 10.1002/0471227617.EOC205, 2003
480. Bertini, I., Capozzi, F., and Luchinat, C., Electronic isomerism in oxidized HiPIPs revisited, **ACS series**, 858, 272-286, 2003

481. Bertini, I., Luchinat, C., Turano, P., Battaini, G., and Casella, L., The magnetic properties of myoglobin as studied by NMR spectroscopy., **Chemistry - A European Journal**, 9, 2316-2322, 2003 (IF 4.238).
482. Bertini, I., Luchinat, C., Nerinovski, K., Parigi, G., Cross, M., Xiao, Z., and Wedd, A. G., Application of NMRD to hydration of rubredoxin and a variant containing a (Cys-S)₃Fe^{III}(OH) site., **Biophys.J.**, 84, 545-551, 2003 (IF 4.643).
483. Bertini, I. and Rosato, A., Bioinorganic chemistry in the post-genomic era., **Proc.Natl.Acad.Sci.USA**, 100, 3601-3604, 1-4-2003 (IF 10.700).
484. Shipp, E., Cantini, F., Bertini, I., Valentine, J. S., and Banci, L., 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 (IF 4.064).
485. 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 (IF 3.922).
486. Andreini, C., Bertini, I., and Rosato, A., A hint to search for metalloproteins in gene banks, **Bioinformatics**, 20, 1373-1380, 2004 (IF 6.701).
487. Andreini, C., Banci, L., Bertini, I., Luchinat, C., and Rosato, A., A bioinformatic comparison of structures and homology-models of matrix metalloproteinases, **J.Proteome Res.**, 3, 21-31, 2004 (IF 5.611).
488. 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, 47998-48003, 2004 (IF 6.482).
489. 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 (IF 5.993).
490. Arnesano, F., Banci, L., Bertini, I., and Ciofi-Baffoni, S., Perspectives in inorganic structural genomics: a trafficking route for copper, **Eur.J.Inorg.Chem.**, 2004, 1583-1593, 2004 (IF 2.482).
491. Arnesano, F. and Bertini, I., Molecular basis of metal-ion selectivity and ultrasensitivity of metalloregulatory proteins, **Chem.Tracts**, 17, 2004
492. 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 (IF 6.516).
493. Babini, E., Bertini, I., Capozzi, F., Del Bianco, C., Holleeder, D., Kiss, T., Luchinat, C., and Quattrone, A., Solution structure of human b-parvalbumin and structural comparison with its paralog a-parvalbumin and with their rat orthologs., **Biochemistry**, 43, 16076-16085, 2004 (IF 3.922).
494. 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 (IF 3.922).

495. Banci, L., Bertini, I., Ciofi-Baffoni, S., Su, X. C., Borrelly, G. P., and Robinson, N. J., Solution structures of a cyanobacterial metallochaperone: insight into an atypical copper-binding motif, **J.Biol.Chem.**, 279, 27502-27510, 25-6-2004
496. Banci, L., Bertini, I., Cavallaro, G., Giachetti, A., Luchinat, C., and Parigi, G., Paramagnetism-based restraints for Xplor-NIH, **J.Biomol.NMR**, 28, 249-261, 2004 (IF 2.420).
497. 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**, 43, 3396-3403, 2004 (IF 3.922).
498. Banci, L., Bertini, I., Cantini, F., Ciofi-Baffoni, S., Gonnelli, L., and Mangani, S., Solution structure of Cox11: a novel type of b-immunoglobulin-like fold involved in CuB site formation of cytochrome *c* oxidase, **J.Biol.Chem.**, 279, 34833-34839, 2004 (IF 6.482).
499. Bartalesi, I., Bertini, I., Di Rocco, G., Ranieri, A., Rosato, A., Vanarotti, M., Viezzoli, M. S., and Vasos, P. R., Protein stability and mutations in the axial methionine loop of a minimal cytochrome *c*, **J.Biol.Inorg.Chem.**, 5, 600-608, 2004 (IF 3.905).
500. 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 (IF 2.343).
501. 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 (IF 3.905).
502. Bertini, I., Rosato, A., and Turano, P., Cytochrome *c* folding/unfolding: a unifying picture. (In honor of Prof. H. Ogoshi), **J.Porph.Phtal.**, 8, 238-245, 2004 (IF 1.438).
503. Bertini, I., Felli, I. C., Kümmerle, R., Luchinat, C., and Pierattelli, R., ^{13}C - ^{13}C NOESY: a constructive use of ^{13}C - ^{13}C spin-diffusion, **J.Biomol.NMR**, 30, 245-251, 2004 (IF 2.420).
504. Bertini, I., Felli, I. C., Kümmerle, R., Moskau, D., and Pierattelli, R., ^{13}C - ^{13}C NOESY: an attractive alternative for studying large macromolecules, **J.Am.Chem.Soc.**, 126, 464-465, 2004 (IF 6.516).
505. Bertini, I., Turano, P., Vasos, P. R., Chevance, S., Bondon, A., and Simonneaux, G., Cytochrome *c* and SDS: a molten globule protein with altered axial ligation., **J.Mol.Biol.**, 336, 489-496, 2004 (IF 5.259).
506. Bertini, I., Calderone, V., Fragai, M., Luchinat, C., Mangani, S., and Terni, B., Crystal structure of the catalytic domain of human matrix metalloproteinase 10, **J.Mol.Biol.**, 336, 707-716, 2004 (IF 5.359).
507. 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 (IF 3.313).
508. Bertini, I., Provenzani, A., Viezzoli, M. S., Pieper, D. H., and Timmis, K. N., NMR spectroscopy as a tool to investigate the degradation of aromatic compounds by a *pseudomonas putida* strain., **Magn.Reson.Chem.**, 41, 615-621, 2004 (IF 1.265).
509. Bertini, I. and Rosato, A., A genomic frontier in bioinorganic chemistry, **Chem.Lett.**, 33, 946-951, 2004 (IF 1.579).

510. Bertini, I., Duma, L., Felli, I. C., Fey, M., Luchinat, C., Pierattelli, R., and Vasos, P. R., A heteronuclear direct detection NMR experiment for protein backbone assignment, **Angew.Chem.Int.Ed.**, 43, 2257-2259, 2004 (IF 8.427).
511. 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 (IF 10.272).
512. 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, 2254-2256, 2004 (IF 8.427).
513. Bertini, I. and Pierattelli, R., Copper(II) proteins are amenable for NMR investigation, **Pure Appl.Chem.**, 76, 321-333, 2004 (IF 1.471).
514. Desvaux, H., Kümmelre, R., Kowalewski, J., Luchinat, C., and Bertini, I., Direct measurement of dynamic frequency shift of cross-correlation in ¹⁵N enriched proteins, **Chem.Phys.Chem.**, 5, 959-965, 2004 (IF 2.070).
515. Andreini, C., Banci, L., Bertini, I., Elmi, S., and Rosato, A., Comparative analysis of the ADAM and ADAMTS families, **J.Proteome Res.**, 4, 881-888, 2005 (IF 6.917).
516. Arnesano, F., Balatri, E., Banci, L., Bertini, I., and Winge, D. R., Folding studies of Cox17 reveal an important interplay of cysteine oxidation and copper binding, **Structure**, 13, 713-722, 2005 (IF 5.993).
517. Arnesano, F., Banci, L., Bertini, I., and Martinelli, M., Ortholog search of proteins involved in copper delivery to Cytochrome c Oxidase and functional analysis of paralogs and gene neighbors by genomic context, **J.Proteome Res.**, 4, 63-70, 2005 (IF 6.917).
518. Arnesano, F., Banci, L., Bertini, I., Fantoni, A., Tenori, L., and Viezzoli, M. S., Structural interplay between calcium(II) and copper(II) binding to S100A13 protein, **Angew.Chem.Int.Ed Engl.**, 44, 6341-6344, 2005
519. Babini, E., Bertini, I., Capozzi, F., Luchinat, C., Quattrone, A., and Turano, M., Principal component analysis of a comprehensive structural database of EF-hand domains to describe the conformational freedom within the EF-hand superfamily, **J.Proteome Res.**, 4, 1961-1971, 2005 (IF 6.917).
520. Banci, L., Bertini, I., Cantini, F., Chasapis, C., Hadjiliadis, N., and Rosato, A., A NMR study of the interaction of a three-domain construct of ATP7A with copper(I) and copper(I)-HAH1: the interplay of domains, **J.Biol.Chem.**, 280, 38259-38263, 2005 (IF 6.355).
521. Banci, L., Bertini, I., Calderone, V., Cramaro, F., Del Conte, R., Fantoni, A., Mangani, S., Quattrone, A., and Viezzoli, M. S., A prokaryotic superoxide dismutase paralog lacking two Cu ligands: from largely unstructured in solution to ordered in the crystal, **Proc.Natl.Acad.Sci.USA**, 102, 7541-7546, 2005 (IF 10.272).
522. Banci, L., Bertini, I., Felli, I. C., and Sarrou, J., Backbone-only restraints for fast determination of the protein fold: The role of paramagnetism-based restraints. Cytochrome b(562) as an example, **J.Magn.Reson.**, 172, 191-200, 2005 (IF 2.461).
523. Banci, L., Bertini, I., D'Amelio, N., Gaggelli, E., Libralesso, E., Matecko, I., Turano, P., and Valentine, J. S., Fully metallated S134N Cu,Zn-Superoxide Dismutase displays abnormal

- mobility and intermolecular contacts in solution, **J.Biol.Chem.**, 280, 35815-35821, 2005 (IF 6.355).
524. Banci, L., Bertini, I., Ciofi-Baffoni, S., Katsari, E., Katsaros, N., Kubicek, K., and Mangani, S., A copper(I) protein possibly involved in the assembly of CuA center of bacterial cytochrome c oxidase., **Proc.Natl.Acad.Sci.USA**, 102, 3994-3999, 2005 (IF 10.272).
525. Banci, L., Bertini, I., and Mangani, S., Integration of XAS and NMR techniques for the structure determination of metalloproteins. Examples from the study of copper transport proteins, **J.Synchrotron Rad.**, 12, 94-94, 2005 (IF 1.144).
526. Banci, L., Bertini, I., Chasapis, C., Ciofi-Baffoni, S., Hadjiliadis, N., and Rosato, A., An NMR study of the interaction between the human copper(I) chaperone and the second and fifth metal-binding domains of the Menkes protein, **FEBS J.**, 272, 865-871, 2005 (IF 3.609).
527. Banci, L., Bertini, I., Cantini, F., Migliardi, M., Rosato, A., and Wang, S., An atomic level investigation of the disease-causing A629P mutant of the Menkes protein ATP7A, **J.Mol.Biol.**, 352, 409-417, 2005 (IF 5.542).
528. Banci, L., Benvenuti, M., Bertini, I., Cabelli, D., Calderone, V., Fantoni, A., Mangani, S., Migliardi, M., and Viezzoli, M. S., From an inactive prokaryotic SOD homolog to an active protein through site directed mutagenesis, **J.Am.Chem.Soc.**, 127, 13287-13292, 2005 (IF 6.903).
529. Bermel, W., Bertini, I., Duma, L., Emsley, L., Felli, I. C., Pierattelli, R., and Vasos, P. R., Complete assignment of heteronuclear protein resonances by protonless NMR spectroscopy, **Angew.Chem.Int.Ed.**, 44, 3089-3092, 2005 (IF 9.161).
530. Bermel, W., Bertini, I., Felli, I. C., Pierattelli, R., and Vasos, P. R., A selective experiment for the sequential protein backbone assignment from 3D heteronuclear spectra, **J.Magn.Reson.**, 172, 324-328, 2005 (IF 2.461).
531. Bertini, I., Jiménez, B., Piccioli, M., and Poggi, L., Asymmetry in ^{13}C - ^{13}C COSY spectra identifies geometry in paramagnetic proteins, **J.Am.Chem.Soc.**, 127, 12216-12217, 2005 (IF 6.903).
532. Bertini, I., Luchinat, C., Parigi, G., and Pierattelli, R., NMR of paramagnetic metalloproteins, **ChemBioChem**, 6, 1536-1549, 2005 (IF 3.474).
533. Bertini, I., Luchinat, C., and Parigi, G., ^1H NMRD profiles of paramagnetic complexes and metalloproteins, **Adv.Inorg.Chem.**, 57, 105-172, 2005 (IF 3.769).
534. Bertini, I., Gupta, Y. K., Luchinat, C., Parigi, G., Schlörb, C., and Schwalbe, H., NMR spectroscopic detection of protein protons and longitudinal relaxation rates between 0.01 and 50 MHz, **Angew.Chem.Int.Ed.**, 44, 2223-2225, 2005 (IF 9.161).
535. Bertini, I., Calderone, V., Cosenza, M., Fragai, M., Lee, Y.-M., Luchinat, C., Mangani, S., Terni, B., and Turano, P., Conformational variability of MMPs: beyond a single 3D structure, **Proc.Natl.Acad.Sci.USA**, 102, 5334-5339, 2005 (IF 10.272).
536. Bertini, I., Fragai, M., Giachetti, A., Luchinat, C., Maletta, M., Parigi, G., and Yeo, K. J., Combining in silico tools and NMR data to validate protein-ligand structural models: application to matrix metalloproteinases, **J.Med.Chem.**, 48, 7544-7559, 2005 (IF 5.076).

537. Bertini, I., Cavallaro, G., and Rosato, A., A structural model for the adduct between cytochrome c and cytochrome c oxidase, **J.Biol.Inorg.Chem.**, 10, 613-624, 2005 (IF 3.300).
538. Bertini, I., Jiménez, B., and Piccioli, M., ^{13}C direct detected experiments: optimisation to paramagnetic signals, **J.Magn.Reson.**, 174, 125-132, 2005 (IF 2.461).
539. Ab, E., Atkinson, A. R., Banci, L., Bertini, I., Ciofi-Baffoni, S., Brunner, K., Diercks, T., Dötsch, V., Engelke, F., Folkers, G., Griesinger, C., Gronwald, W., Gunther, H., Habeck, M., de Jong, R., Kalbitzer, H. R., Kieffer, B., Leeflang, B. R., Loss, S., Luchinat, C., Marquardsen, T., Moskau, D., Neidig, K. P., Nilges, M., Piccioli, M., Pierattelli, R., Rieping, W., Schippmann, T., Schwalbe, H., Trave, G., Trenner, J. M., Wohner, J., Zweckstetter, M., and Kaptein, R., NMR in structural proteomics, **Acta Crystallogr D Biol Crystallogr**, 62, 1161-, 2006 (IF 1.401).
540. Achila, D., Banci, L., Bertini, I., Bunce, J., Ciofi-Baffoni, S., and Huffman, D. L., Structure of human Wilson protein domains 5 and 6 and their interplay with domain 4 and the copper chaperone HAH1 in copper uptake, **Proc.Natl.Acad.Sci.USA**, 103, 5729-5734, 2006 (IF 10.231).
541. Albeck, S., Alzari, P., Andreini, C., Banci, L., Berry, I. M., Bertini, I., Cambillau, C., Canard, B., Carter, L., Cohen, S., Diprose, JM, Dym, O., Esnouf, RM, Felder, C., Ferron, F., Guillemot, F., Hamer, R., Ben Jelloul, M., Laskowski, RA, Laurent, T., Longhi, S., Lopez, R., Luchinat, C., Malet, H., Mochel, T., Morris, R. J., Moulinier, L., Oinn, T., Pajon, A., Peleg, Y., Perrakis, A., Poch, O., Prilusky, J., Rachedi, A., Ripp, R., Rosato, A., Silman, I., Stuard, D. I., Sussman, J. L., Thierry, J. C., Thompson, J. D., Thornton, J. M., Unger, T., Vaughan, B., Vranken, W., Watson, J. D., Whamond, G., and Herik, K., SPINE bioinformatics and data-management aspects of high-throughput structural biology, **Acta Crystallogr D Biol Crystallogr**, 62, 1184-1195, 2006 (IF 1.401).
542. Andreini, C., Banci, L., Bertini, I., and Rosato, A., Counting the zinc proteins encoded in the human genome, **J.Proteome Res.**, 5, 196-201, 2006 (IF 6.901).
543. Andreini, C., Banci, L., Bertini, I., and Rosato, A., Zinc through the three domains of life, **J.Proteome Res.**, 5, 3173-3178, 2006 (IF 6.901).
544. Arnesano, F., Banci, L., Bertini, I., Capozzi, F., Ciurli, S., Luchinat, C., Mangani, S., Ciofi-Baffoni, S., Rosato, A., Turano, P., and Viezzoli, M. S., An Italian contribution to structural genomics: understanding metalloproteins., **Coord.Chem.Rev.**, 250, 1419-1450, 2006 (IF 9.779).
545. Babini, E., Bertini, I., Capozzi, F., Chirivino, E., and Luchinat, C., A structural and dynamic characterization of the EF-hand protein CLSP, **Structure**, 14, 1029-1038, 2006 (IF 5.543).
546. Balayssac, S., Bertini, I., Luchinat, C., Parigi, G., and Piccioli, M., ^{13}C direct detected NMR increases the detectability of residual dipolar couplings, **J.Am.Chem.Soc.**, 128, 15042-15043, 2006 (IF 7.419).
547. Banci, L., Bertini, I., Calderone, V., Ciofi-Baffoni, S., Mangani, S., Martinelli, M., Palumaa, P., and Wang, S., A hint for the function of human Sco1 from different structures, **Proc.Natl.Acad.Sci.USA**, 103, 8595-8600, 2006 (IF 10.231).
548. Banci, L., Bertini, I., Cantini, F., Felli, I. C., Gonnelli, L., Hadjiliadis, N., Pierattelli, R., Rosato, A., and Voulgaris, P., The Atx1-Ccc2 complex is a metal-mediated protein-protein interaction, **Nat.Chem.Biol.**, 2, 367-368, 2006

549. Banci, L., Bertini, I., Ciofi-Baffoni, S., Kandias, N. G., Spyroulias, G. A., Su, X. C., Robinson, N. J., and Vanarotti, M., The delivery of copper for thylakoid import observed by NMR, **Proc.Natl.Acad.Sci.USA**, 103, 8325-, 2006 (IF 10.231).
550. Banci, L., Bertini, I., Cusack, S., deJon, R. N., Heinemann, U., Jones, E. Y., Kozielski, F., Maskos, K., Messerschmidt, A., Owens, R., Perrakis, A., Poterszman, A., Schneider, G., Siebold, C., Silman, I., Sixman, T., Stewart-Jones, G., Sussman, J. L., Thierry, J. C., and Moras, D., First steps towards effective methods in exploiting high-throughput technologies for the determination of human protein structures of high biomedical value., **Acta Crystallogr D Biol Crystallogr**, 62, 1208-1217, 2006 (IF 1.401).
551. Banci, L., Bertini, I., Ciofi-Baffoni, S., Su, X. C., Miras, R., Bal, N., Mintz, E., Catty, P., Shokes, J. E., and Scott, R. A., Structural basis for metal binding specificity: the N-terminal cadmium binding domain of the P1-type ATPase CadA, **J.Mol.Biol.**, 356, 638-650, 2006 (IF 5.542).
552. Banci, L., Bertini, I., Cantini, F., Della Malva, N., Rosato, A., Herrmann, T., and Wüthrich, K., Solution structure and intermolecular interactions of the third metal-binding domain of ATP7A, the Menkes disease protein, **J.Biol.Chem.**, 281, 29141-29147, 2006 (IF 5.854).
553. Banci, L., Bertini, I., Cantini, F., D'Amelio, N., and Gaggelli, E., Human SOD1 Before Harboring the Catalytic Metal: Solution Structure of Copper-Depleted, Disulfide-Reduced Form., **J.Biol.Chem.**, 281, 2333-2337, 2006 (IF 5.854).
554. Bermel, W., Bertini, I., Felli, I. C., Piccioli, M., and Pierattelli, R., ^{13}C -detected protonless NMR spectroscopy of proteins in solution, **Progr.NMR Spectrosc.**, 48, 25-45, 2006 (IF 6.462).
555. Bermel, W., Bertini, I., Felli, I. C., Lee, Y.-M., Luchinat, C., and Pierattelli, R., Protonless NMR experiments for sequence-specific assignment of backbone nuclei in unfolded proteins, **J.Am.Chem.Soc.**, 128, 3918-3919, 2006 (IF 7.419).
556. Bermel, W., Bertini, I., Felli, I. C., Kümmeler, R., and Pierattelli, R., Novel ^{13}C direct detection experiments, including extension to the third dimension, to perform the complete assignment of proteins, **J.Magn.Reson.**, 178, 56-64, 2006 (IF 2.418).
557. Bertini, I., Felli, I. C., Gonnelli, L., Pierattelli, R., Spyranti, Z., and Spyroulias, G. A., Mapping protein-protein interaction by $^{13}\text{C}'$ -detected heteronuclear NMR spectroscopy, **J.Biomol.NMR**, 36, 111-122, 2006 (IF 2.18).
558. Bertini, I., Cavallaro, G., and Rosato, A., Cytochrome c: occurrence and functions, **Chem.Rev.**, 106, 90-115, 2006 (IF 20.869).
559. Bertini, I., Grassi, E., Luchinat, C., Quattrone, A., and Saccenti, E., Monomorphism of human Cytochrome c, **Genomics**, 88, 669-672, 2006 (IF 3.181).
560. Bertini, I., Calderone, V., Fragai, M., Luchinat, C., and Maletta, M., Snapshots of the reaction mechanism of Matrix metalloproteinases, **Angew.Chem.Int.Ed.**, 45, 7952-7955, 2006 (IF 9.596).
561. Caillet-Saguy, C., Delepierre, M., Lecroisey, A., Bertini, I., Piccioli, M., and Turano, P., Direct detected ^{13}C NMR to investigate the Iron(III) hemophore HasA, **J.Am.Chem.Soc.**, 128, 150-158, 2006 (IF 7.419).
562. Fogg, M. J., Alzari, P., Bahar, M., Bertini, I., Betton, J. M., Burmeister, W. P., Cambillau, C., Canard, B., Carrondo, M. A., Coll, M., Daenke, S., Dym, O., Emgloff, M. P., Enguita, F.

- J., Gerlof, A., Haouz, A., Jones, T. A., Ma, Q. F., Manica, P., Migliardi, M., Nordlund, P., Owens, R. J., Peleg, Y., Schneider, G., Schnell, R., Stuart, D. I., Tarbouriech, N., Unge, T., Wilkinson, A. J., Wilmanns, M., Wilson, K. S., Zimhony, O., and Grimes, J. M., Application of the use of high-throughput technologies to the determination of protein structures of bacterial and viral pathogens, **Acta Crystallogr D Biol Crystallogr**, 62, 1196-1207, 2006
563. Alcaraz, L. A., Banci, L., Bertini, I., Cantini, F., Donaire, A., and Gonnelli, L., MMP-inhibitor interaction: the solution structure of the catalytic domain of human matrix metalloproteinase-3 with three inhibitors, **J.Biol.Inorg.Chem.**, 12, 1197-1206, 2007 (IF 3.300).
564. Andreini, C., Banci, L., Bertini, I., Elmi, S., and Rosato, A., Non-heme iron through the three domains of life, **Proteins**, 67, 317-324, 2007 (IF 3.73).
565. Arendt, Y., Banci, L., Bertini, I., Cantini, F., Cozzi, R., Del Conte, R., and Gonnelli, L., Catalytic domain of MMP20 (Enamelysin) - the NMR structure of a new Matrix metalloproteinase, **FEBS Lett.**, 581, 4723-4726, 2007 (IF 3.37).
566. Assfalg, M., Bertini, I., Del Conte, R., Giachetti, A., and Turano, P., Cytochrome c and Organic Molecules: the Solution Structure of the Para-Aminophenol Adduct, **Biochemistry**, 46, 6232-6238, 2007 (IF 3.63).
567. Balayssac, S., Bertini, I., Lelli, M., Luchinat, C., Maletta, M., and Yeo, K. J., Paramagnetic ions provide precious structural restraints in solid-state NMR of proteins, **J.Am.Chem.Soc.**, 129, 2218-2219, 2007 (IF 7.696).
568. Balayssac, S., Bertini, I., Falber, K., Fragai, M., Jehle, S., Lelli, M., Luchinat, C., Oschkinat, H., and Yeo, K. J., Solid-state NMR of matrix metalloproteinase 12: an approach complementary to solution NMR, **ChemBioChem**, 8, 486-489, 2007 (IF 4.100).
569. Banci, L., Bertini, I., Ciofi-Baffoni, S., Gerohanassis, I. P., Leontari, I., Martinelli, M., and Wang, S., A structural characterization of human Sco2, **Structure**, 15, 1132-1140, 2007 (IF 5.74).
570. Banci, L., Bertini, I., Cavallaro, G., and Rosato, A., The functions of Sco proteins from genome-based analysis, **J.Proteome Res.**, 6, 1568-1579, 2007 (IF 5.15).
571. Banci, L., Bertini, I., Chasapis, C., Rosato, A., and Tenori, L., Interaction of the two soluble metal-binding domains of yeast Ccc2 with copper(I)-Atx1., **Biochem.Biophys.Res.Commun.**, 364, 645-649, 2007 (IF 2.86).
572. Banci, L., Bertini, I., Girotto, S., Martinelli, M., Vieru, M., Whitelegge, JP, Durazo, A., and Valentine, J. S., Metal-free SOD1 forms amyloid-like oligomers: a possible general mechanism for familial ALS; **Proc.Natl.Acad.Sci.USA**, 104, 11263-11267, 2007 (IF 9.643).
573. Banci, L., Bertini, I., Cantini, F., Ciofi-Baffoni, S., Cavet, J. S., Dennison, C., Graham, A. I., Harvie, D. R., and Robinson, N. J., NMR structural analysis of cadmium-sensing by winged helix repressor CMTR, **J.Biol.Chem.**, 282, 30181-30188, 2007 (IF 5.81).
574. Banci, L., Bertini, I., Ciofi-Baffoni, S., Boelens, R., Bonvin, A. M., and van Dijk, A. D. J., Modeling protein-protein complexes involved in the cytochrome *c* oxidase copper-delivery pathway, **J.Proteome Res.**, 6, 1530-1539, 2007 (IF 5.15).

575. Banci, L., Bertini, I., Cantini, F., Della Malva, N., Migliardi, M., and Rosato, A., The different intermolecular interactions of the soluble copper-binding domains of the Menkes protein, ATP7A, **J.Biol.Chem.**, 282, 23140-23146, 2007 (IF 5.81).
576. Banci, L., Bertini, I., D'Amelio, N., Libralesso, E., Turano, P., and Valentine, J. S., Metallation of the ALS-Mutant G37R SOD1 Apoprotein Restores its Structural and Dynamical Properties in Solution to those of Metallated Wild Type SOD1, **Biochemistry**, 46, 9953-9962, 2007 (IF 3.63).
577. Banci, L., Bertini, I., Ciofi-Baffoni, S., Leontari, I., Martinelli, M., Palumaa, P., Sillard, R., and Wang, S., Human Sco1 functional studies and pathological implications of the P174L mutant, **Proc.Natl.Acad.Sci.USA**, 104, 15-20, 2007 (IF 9.643).
578. Bertini, I., Gupta, Y. K., Luchinat, C., Parigi, G., Peana, M., Sgheri, L., and Yuan, J., Paramagnetism-Based NMR Restraints Provide Maximum Allowed Probabilities for the Different Conformations of Partially Independent Protein Domains, **J.Am.Chem.Soc.**, 129, 12786-12794, 2007 (IF 7.696).
579. Bertini, I. and Rosato, A., From genes to metalloproteins: a bioinformatic approach, **Eur.J.Inorg.Chem.**, 18, 2546-2555, 2007 (IF 2.7).
580. Bertini, I., Calderone, V., Fragai, M., Giachetti, A., Loconte, M., Luchinat, C., Maletta, M., Nativi, C., and Yeo, K. J., Exploring the subtleties of drug-receptor interactions: the case of matrix metalloproteinases, **J.Am.Chem.Soc.**, 129, 2466-2475, 2007 (IF 7.696).
581. Bertini, I., Felli, I. C., Luchinat, C., Parigi, G., and Pierattelli, R., Towards a protocol for solution structure determination of copper(II) proteins: the case of Cu(II)Zn(II) superoxide dismutase, **ChemBioChem**, 8, 1422-1429, 2007 (IF 4.100).
582. Bertini, I., Cavallaro, G., and Rosato, A., Evolution of mitochondrial-type cytochrome *c* domains and of the protein machinery for their assembly, **J.Inorg.Biochem.**, 101, 1798-1811, 2007 (IF 2.423).
583. Claudino, W. M., Quattrone, A., Biganzoli, L., Pestrin, M., Bertini, I., and Di Leo, A., Metabolomics: Available results, current research projects in breast cancer, and future applications, **J.Clin.Oncol.**, 25, 2840-2846, 1-7-2007
584. Coyne, H. J., Ciofi-Baffoni, S., Banci, L., Bertini, I., Zhang, L., Graham, N. G., and Winge, D. R., The characterization and the role of zinc binding in yeast cox4, **J.Biol.Chem.**, 282, 8926-8934, 2007 (IF 5.81).
585. Matzapetakis, M., Turano, P., Theil, E. C., and Bertini, I., ^{13}C - ^{13}C NOESY spectra of a 480 kDa protein: solution NMR of ferritin, **J.Biomol.NMR**, 38, 237-242, 2007 (IF 1.79).
586. Pintacuda, G., Giraud, N., Pierattelli, R., Böckmann, A., Bertini, I., and Emsley, L., Solid-state NMR of a paramagnetic protein: assignment and study of human dimeric oxidized Cu(II), Zn(II) superoxide dismutase, **Angew.Chem.Int.Ed.**, 46, 1079-1082, 2007 (IF 10.23).
587. Stiefel, E. I., Bioinorganic chemistry and the biogeochemical cycles, in: Biological Inorganic Chemistry, Bertini, I., Gray, H. B., Stiefel, E. I., and Valentine, J. S., 7, <[05] Date, primary>
588. Abriata, L. A., Banci, L., Bertini, I., Ciofi-Baffoni, S., Gkazonis, P., Spyroulias, G. A., Vila, A. J., and Wang, S., Mechanism of Cu(A) assembly, **Nat.Chem.Biol.**, 4, 599-601, 2008 (IF 13.68).

589. Andreini, C., Bertini, I., Cavallaro, G., Holliday, G. L., and Thornton, J. M., Metal ions in biological catalysis: from enzyme databases to general principles, **J.Biol.Inorg.Chem.**, 13, 1205-1218, 2008 (IF 3.325).
590. Andreini, C., Banci, L., Bertini, I., and Rosato, A., Occurrence of copper through the three domains of life: a bioinformatic approach, **J.Proteome Res.**, 1, 209-216, 2008 (IF 5.675).
591. Assfalg, M., Bertini, I., Colangiuli, D., Luchinat, C., Schafer, H., Schutz, B., and Spraul, M., Evidence of different metabolic phenotypes in humans, **Proc.Natl.Acad.Sci.USA**, 105, 1420-1424, 5-2-2008
592. Balayssac, S., Bertini, I., Bhaumik, A., Lelli, M., and Luchinat, C., Paramagnetic shifts in solid-state NMR of proteins to elicit structural information., **Proc.Natl.Acad.Sci.USA**, 105, 17284-17289, 2008 (IF 9.598).
593. Banci, L., Bertini, I., Ciofi-Baffoni, S., Janicka, A., Martinelli, M., Kozlowski, H., and Palumaa, P., A structural-dynamical characterization of human Cox17, **J.Biol.Chem.**, 283, 7912-7920, 2008 (IF 5.81).
594. Banci, L., Bertini, I., Cantini, F., Rosenzweig, A. C., and Yatsunyk, L. A., Metal binding domains 3 and 4 of the Wilson disease protein: solution structure and interaction with the copper(I) chaperone HAH1, **Biochemistry**, 47, 7423-7429, 2008 (IF 3.368).
595. Banci, L., Bertini, I., Ciofi-Baffoni, S., Hadjiloi, T., Martinelli, M., and Palumaa, P., Mitochondrial copper(I) transfer from Cox17 to Sco1 is coupled to electron transfer, **Proc.Natl.Acad.Sci.USA**, 105, 6803-6808, 2008 (IF 9.598).
596. Banci, L., Bertini, I., Boca, M., Girotto, S., Martinelli, M., Valentine, J. S., and Vieru, M., SOD1 and amyotrophic lateral sclerosis: mutations and oligomerization, **Plos ONE**, 3, e1677-, 2008
597. Bermel, W., Bertini, I., Felli, I. C., Kümmerle, R., and Pierattelli, R., Pursuing direct ^{13}C detection for biomolecular NMR in solution, **Bruker Spin Report**, 159/160, 26-31, 2008
598. Bertini, I. and Cavallaro, G., Metals in the "omics" world: copper homeostasis and cytochrome c oxidase assembly in a new light, **J.Biol.Inorg.Chem.**, 13, 3-14, 2008 (IF 3.325).
599. Bertini, I. and Rosato, A., Menkes disease, **Cell.Mol.Life Sci.**, 65, 89-91, 2008 (IF 5.239).
600. Bertini, I., Calderone, V., Fragai, M., Jaiswal, R., Luchinat, C., Melikian, M., Mylonas, E., and Svergun, D., Evidence of reciprocal reorientation of the catalytic and hemopexin-like domains of full-length MMP-12, **J.Am.Chem.Soc.**, 130, 7011-7021, 2008 (IF 7.885).
601. Bertini, I., Luchinat, C., Parigi, G., and Pierattelli, R., NMR spectroscopy of paramagnetic metalloproteins, in: Encyclopedia of Chemical Biology, Wiley, <[05] Date, primary>
602. Bertini, I., Luchinat, C., Parigi, G., and Pierattelli, R., Perspectives in NMR of paramagnetic proteins, **Dalton Trans.**, 2008, 3782-3790, 2008 (IF 3.212).
603. Bertini, I., Jiménez, B., Pierattelli, R., Wedd, A. G., and Xiao, Z., Protonless ^{13}C direct detection NMR: Characterization of the 37 kiloDalton trimeric protein CutA1, **Proteins Struct.Funct.Genet.**, 70, 1196-1205, 2008 (IF 3.730).
604. Bertini, I., Fragai, M., Luchinat, C., and Talluri, E., Water-based ligand screening for paramagnetic metalloproteins, **Angew.Chem.Int.Ed.**, 47, 4533-4537, 2008 (IF 10.031).

605. Csizmok, V., Felli, I. C., Tompa, P., Banci, L., and Bertini, I., Structural and dynamic characterization of intrinsically disordered human securin by NMR., **J.Am.Chem.Soc.**, 130, 16873-16879, 2008 (IF 7.885).
606. Pellecchia, M., Bertini, I., Cowburn, D., Dalvit, C., Giralt, E., Jahnke, W., James, T. L., Homans, S. W., Kessler, H., Luchinat, C., Meyer, B., Oschkinat, H., Peng, J., Schwalbe, H., and Siegal, G., Perspectives on NMR in drug discovery: a technique comes of age, **Nature Rev.Drug Discov.**, 7, 738-745, 2008 (IF 23.308).
607. Andreini, C., Bertini, I., Cavallaro, G., Holliday, G. L., and Thornton, J. M., Metal-MACiE: a database of metals involved in biological catalysis., **Bioinformatics**, 25, 2088-2089, 2009 (IF 5.039).
608. Andreini, C., Bertini, I., and Rosato, A., Metalloproteomes: a bioinformatic approach., **Acc.Chem.Res.**, 42, 1471-1479, 2009 (IF 12.176).
609. Andreini, C., Bertini, I., Cavallaro, G., Najmanovich, R. J., and Thornton, J. M., Structural analysis of metal sites in proteins: non-heme iron sites as a case study, **J.Mol.Biol.**, 388, 356-380, 2009 (IF 4.146).
610. Banci, L., Bertini, I., and Ciofi-Baffoni, S., Copper trafficking in biology: an NMR approach, **HFSP J.**, 3, 165-175, 2009 (IF).
611. Banci, L., Bertini, I., Boca, M., Calderone, V., Cantini, F., Giroto, S., and Vieru, M., Structural and dynamic aspects related to oligomerization of apo SOD1 and its mutants, **Proc.Natl.Acad.Sci.U.S.A.**, 106, 6980-6985, 28-4-2009
612. Banci, L., Bertini, I., Cefaro, C., Ciofi-Baffoni, S., Gallo, A., Martinelli, M., Sideris, D. P., Katrakili, N., and Tokatlidis, K., MIA40 is an oxidoreductase that catalyzes oxidative protein folding in mitochondria, **Nat.Struct.Mol.Biol.**, 16, 198-206, 2009 (IF 10.987).
613. Banci, L., Bertini, I., Ciofi-Baffoni, S., and Tokatlidis, K., The coiled coil-helix-coiled coil-helix proteins may be redox proteins, **FEBS Lett.**, 11, 1699-1702, 2-4-2009 (IF 3.264).
614. Banci, L., Bertini, I., Calderone, V., Della Malva, N., Felli, I. C., Neri, S., Pavelkova, A., and Rosato, A., Copper(I)-mediated protein-protein interactions result from suboptimal interaction surfaces, **Biochem.J.**, 422, 37-42, 2009 (IF 4.371).
615. Banci, L., Bertini, I., Cantini, F., Massagni, C., Migliardi, M., and Rosato, A., An NMR study of the interaction of the N-terminal cytoplasmic tail of the Wilson disease protein with copper(I)-HAH1, **J.Biol.Chem.**, 284, 9354-9360, 2009 (IF 5.520).
616. Banci, L., Bertini, I., Cantini, F., Migliardi, M., Natile, G., Nushi, F., and Rosato, A., Solutions structures of the actuator domain of ATP7A and ATP7B, the menkes and wilson disease proteins, **Biochemistry**, 48, 7849-7855, 2009 (IF 3.379).
617. Bermel, W., Bertini, I., Csizmok, V., Felli, I. C., Pierattelli, R., and Tompa, P., H-start for exclusively heteronuclear NMR spectroscopy: the case of intrinsically disordered proteins., **J.Magn.Reson.**, 198, 275-281, 2009 (IF 2.438).
618. Bermel, W., Bertini, I., Felli, I. C., and Pierattelli, R., Speeding up ¹³C direct detection NMR experiments, **J.Am.Chem.Soc.**, 131, 15339-15345, 2009 (IF 8.091).

619. Bernini, P., Bertini, I., Nepi, S., Saccenti, E., Schaefer, H., Schuetz, B., Spraul, M., and Tenori, L., Individual human phenotypes in metabolic space and time., **J.Proteome Res.**, 8, 4264-4271, 2009 (IF 5.684).
620. Bertini, I., Fragai, M., Luchinat, C., Melikian, M., and Venturi, C., Characterization of the MMP-12-elastin adduct, **Chemistry - A European Journal**, 15, 7842-7845, 2009 (IF 5.454).
621. Bertini, I., Fragai, M., and Luchinat, C., Intra- and Interdomain Flexibility in Matrix Metalloproteinases: Functional Aspects and Drug Design, **Curr.Pharm.Des.**, 15, 3592-3605, 2009 (IF 4.399).
622. Bertini, I., Fragai, M., Luchinat, C., Melikian, M., Mylonas, E., Sarti, N., and Svergun, D., Interdomain flexibility in full-length matrix metalloproteinase-1 (MMP-1), **J.Biol.Chem.**, 284, 12821-12828, 2009 (IF 5.520).
623. Bertini, I., Calderone, V., Fragai, M., Luchinat, C., and Talluri, E., Structural basis of serine/threonine phosphatase inhibition by the archetypal small molecules cantharidin and norcantharidin, **J.Med.Chem.**, 52, 4838-4843, 2009 (IF 4.898).
624. Bertini, I., Calabro, A., De carli, V., Luchinat, C., Nepi, S., Porfirio, B., Renzi, D., Saccenti, E., and Tenori, L., The metabonomic signature of celiac disease, **J.Proteome Res.**, 1, 170-177, 2009 (IF 5.684).
625. Bertini, I., Kursula, P., Luchinat, C., Parigi, G., Vahokoski, J., Willmans, M., and Yuan, J., Accurate solution structures of proteins from X-ray data and minimal set of NMR data: calmodulin peptide complexes as examples., **J.Am.Chem.Soc.**, 131, 5134-5144, 2009 (IF 8.091).
626. Bertini, I., Dasgupta, S., Hu, X., Karavelas, T., Luchinat, C., Parigi, G., and Yuan, J., Solution structure and dynamics of S100A5 in the apo and Ca²⁺-bound states, **J.Biol.Inorg.Chem.**, 14, 1097-1107, 2009 (IF 3.6).
627. Caillet-Saguy, C., Piccioli, M., Turano, P., Izadi-Pruneyre, N., Delepine, M., Bertini, I., and Lecroisey, A., Mapping the Interaction between the Hemophore HasA and its Outer Membrane Receptor HasR using CRINEPT-TROSY NMR Spectroscopy, **J.Am.Chem.Soc.**, 131, 1736-1744, 2009 (IF 8.091).
628. Isaksson, J., Nystroem, S., Derbshire, W., Wallberg, H., Agback, T., Kovacs, H., Bertini, I., Giachetti, A., and Luchinat, C., Does a fast nuclear magnetic resonance spectroscopy- and X-ray crystallography hybrid approach provide reliable structural information of ligand-protein complexes? A case study of metalloproteinases, **J.Med.Chem.**, 52, 1712-1722, 2009 (IF 4.898).
629. Laage, S., Lesage, A., Emsley, L., Bertini, I., Felli, I. C., Pierattelli, R., and Pintacuda, G., Transverse-Dephasing Optimized Homonuclear J-Decoupling in Solid-State NMR Spectroscopy of Uniformly (¹³C)-Labeled Proteins, **J.Am.Chem.Soc.**, 131, 10816-+, 12-8-2009
630. Laage, S., Lesage, A., Emsley, L., Bertini, I., Felli, I. C., Pierattelli, R., and Pintacuda, G., Transverse-dephasing optimized homonuclear J-decoupling in solid-state NMR spectroscopy of uniformly ¹³C-labeled proteins, **J.Am.Chem.Soc.**, 131, 10816-10817, 2009 (IF 8.091).
631. Sideris, D. P., Petrakis, N., Katrakili, N., Mikropoulou, D., Gallo, A., Ciofi-Baffoni, S., Banci, L., Bertini, I., and Tokatlidis, K., A novel intermembrane space-targeting signal docks

- cysteines onto Mia40 during mitochondrial oxidative folding, **J.Cell Biol.**, 187, 1007-1022, 2009 (IF 9.120).
632. Banci, L., Bertini, I., Cefaro, C., Cenacchi, L., Ciofi-Baffoni, S., Felli, I. C., Gallo, A., Gonnelli, L., Luchinat, E., Sideris, D. P., and Tokatlidis, K., Molecular chaperone function of Mia40 triggers consecutive induced folding steps of the substrate in mitochondrial protein import, **Proc.Natl.Acad.Sci.USA**, 107, 20190-20195, 2010 (IF 9.432).
633. Banci, L., Bertini, I., Ciofi-Baffoni, S., Poggi, L., Vanarotti, M., Tottey, S., Waldron, K. J., and Robinson, N. J., NMR structural analysis of the soluble domain of ZiaA-ATPase and the basis of selective interactions with copper metallochaperone Atx1, **J.Biol.Inorg.Chem.**, 15, 87-98, 2010 (IF 3.6).
634. Banci, L., Bertini, I., McGreevy, K. S., and Rosato, A., Molecular recognition in copper trafficking, **Nat.Prod.Rep.**, 27, 695-710, 2010 (IF 7.45).
635. Banci, L., Bertini, I., Cantini, F., and Ciofi-Baffoni, S., Cellular copper distribution: a mechanistic systems biology approach, **Cell.Mol.Life Sci.**, 67, 2563-2589, 2010 (IF 5.511).
636. Banci, L., Bertini, I., Luchinat, C., and Mori, M., NMR in structural proteomics and beyond, **Prog.NMR Spectrosc.**, 56, 247-266, 2010 (IF 6.162).
637. Banci, L., Bertini, I., Cantini, F., Inagaki, S., Migliardi, M., and Rosato, A., The binding mode of ATP revealed by the solution structure of the N-domain of human ATP7A, **J.Biol.Chem.**, 285, 2537-2544, 16-11-2010 (IF 5.520).
638. Banci, L., Bertini, I., Ciofi-Baffoni, S., Kozyreva, T., Zovo, K., and Palumaa, P., Affinity gradients drive copper to cellular destinations, **Nature**, 465, 645-648, 2010 (31.434).
639. Bermel, W., Bertini, I., Felli, I. C., Peruzzini, R., and Pierattelli, R., Exclusively heteronuclear NMR experiments to obtain structural and dynamic information on proteins, **ChemPhysChem**, 11, 689-695, 2010 (IF 3.636).
640. Bertini, I., Bhaumik, A., De Paepe, G., Griffin, R. G., Lelli, M., Lewandowski, J. R., and Luchinat, C., High-Resolution Solid-State NMR Structure of a 17.6 kDa Protein, **J.Am.Chem.Soc.**, 132, 1032-1040, 27-1-2010
641. Bertini, I., Emsley, L., Lelli, M., Luchinat, C., Mao, J., and Pintacuda, G., Ultra-Fast MAS solid-state NMR permits extensive ¹³C and ¹H detection in paramagnetic metalloproteins, **J.Am.Chem.Soc.**, 132, 5558-5559, 2010 (IF 8.580).
642. Bertini, I., Cavallaro, G., and McGreevy, K. S., Cellular copper management - a user's guide, **Coord.Chem.Rev.**, 254, 506-524, 2010 (IF 10.566).
643. Bertini, I., Decaria, L., and Williams, R. J. P., Zinc proteomes, phylogenetics and evolution, **Metalomics**, 2, 706-709, 2010 (IF 0.755).
644. Bertini, I., Giachetti, A., Luchinat, C., Parigi, G., Petoukhov, M. V., Pierattelli, R., Ravera, E., and Svergun, D. I., Conformational space of flexible biological macromolecules from average data, **J.Am.Chem.Soc.**, 132, 13553-13558, 2010 (IF 8.580).
645. Bertini, I., Decaria, L., and Rosato, A., The annotation of full zinc proteomes, **J.Biol.Inorg.Chem.**, 15, 1071-1078, 2010 (IF 3.6).

646. Bertini, I. and Cavallaro, G., Bioinformatics in bioinorganic chemistry, **Metalloomics**, 2, 39-51, 2010
647. Loureiro-Ferreira, N., Wassenaar, T. A., de Vries, S. J., van Dijk, M., van der Schot, G., van der Zwan, J., Boelens, R., Giachetti, A., Carotenuto, D., Rosato, A., Bertini, I., Herrmann, T., Bagaria, A., Zharavin, V., Jonker, H. R., Guentert, P., Schwalbe, H., Vranken, W. F., Dal Pra, S., Mazzuccato, S., Frizziero, M., Traldi, S., Verlato, M., and Bonvin, A. M. J. J., e-NMR gLite grid enabled infrastructure, in: IBERGRID 4th Iberian Grid infrastructure Conference Proceedings, Proen  a, A., Pina, A., Garcia Tobio, J., and Ribeiro, L., 360, <[05] Date, primary>
648. Madl, T., Felli, I. C., Bertini, I., and Sattler, M., Structural analysis of protein interfaces from ¹³C direct-detect paramagnetic relaxation enhancements, **J.Am.Chem.Soc.**, 132, 7285-7287, 2010 (IF 8.580).
649. Turano, P., Lalli, D., Felli, I. C., Theil, E. C., and Bertini, I., NMR reveals a pathway for iron mineral precursors to the central cavity of ferritin, **Proc.Natl.Acad.Sci.USA**, 107, 545-550, 2010 (IF 9.432).
650. Andreini, C., Bertini, I., Cavallaro, G., Decaria, L., and Rosato, A., A simple protocol for the comparative analysis of the structure and occurrence of biochemical pathways across superkingdoms, **J.Chem.Inf.Model.**, 51, 730-738, 2011 (IF 3.822).
651. Babini, E., Bertini, I., Borsi, V., Calderone, V., Hu, X., Luchinat, C., and Parigi, G., Structural characterization of human S100A16, a low affinity calcium binder, **J.Biol.Inorg.Chem.**, 16, 243-256, 2011 (IF 3.287).
652. Banci, L., Bertini, I., Calderone, V., Cefaro, C., Ciofi-Baffoni, S., Gallo, A., Kallergi, E., Lionaki, E., Pozidis, C., and Tokatlidis, K., Molecular recognition and substrate mimicry drive the electron-transfer process between MIA40 and ALR, **Proc.Natl.Acad.Sci.USA**, 108, 4811-4816, 2011 (IF 9.771).
653. Banci, L., Bertini, I., Ciofi-Baffoni, S., Boscaro, F., Chatzi, A., Mikolajczyk, M., Tokatlidis, K., and Winkelmann, J., Anamorsin is a 2Fe2S cluster-containing substrate of the Mia40-dependent mitochondrial protein trapping machinery, **Chem.Biol.**, 18, 794-804, 2011 (IF 5.603).
654. Banci, L., Bertini, I., Ciofi-Baffoni, S., D'Alessandro, A., Jaiswal, D., Marzano, V., Neri, S., Ronci, M., and Urbani, A., Copper exposure effects on yeast mitochondrial proteome, **J.Proteomics**, epub ahead of print, 2011 (IF 3.851).
655. Banci, L., Bertini, I., Cefaro, C., Ciofi-Baffoni, S., and Gallo, A., The functional role of two interhelical disulfide bonds in human Cox17 from a structural perspective, **J.Biol.Chem.**, epub ahead of print, 2011 (IF 5.328).
656. Banci, L., Barbieri, L., Bertini, I., Cantini, F., and Luchinat, E., In-cell NMR in E.coli to monitor maturation steps of hSOD1, **Plos ONE**, 6, e23561-, 2011 (IF 4.411).
657. Banci, L., Bertini, I., Ciofi-Baffoni, S., Kozyreva, T., Mori, M., and Wang, S., SCO proteins are involved in electron transfer processes, **J.Biol.Inorg.Chem.**, 13, 391-403, 2011 (IF 3.287).
658. Banci, L., Bertini, I., Blazevits, O., Cantini, F., Lelli, M., Luchinat, C., Mao, J., and Vieru, M., NMR characterization of a "fibril-ready" state of demetallated wild-type superoxide dismutase, **J.Am.Chem.Soc.**, 133, 345-349, 2011 (IF 9.019).

659. Bernini, P., Bertini, I., Luchinat, C., Nincheri, P., Staderini, S., and Turano, P., Standard operating procedures for pre-analytical handling of blood and urine for metabolomic studies and biobanks, **J.Biomol.NMR**, 49, 231-243, 2011 (IF 3.047).
660. Bernini, P., Bertini, I., Calabro, A., La Marca, G., Lami, G., Luchinat, C., Renzi, D., and Tenori, L., Are patients with potential celiac disease really potential? The answer of metabonomics, **J.Proteome Res.**, 10, 714-721, 2011 (IF 5.460).
661. Bernini, P., Bertini, I., Luchinat, C., Tenori, L., and Tognaccini, A., The cardiovascular risk of healthy individuals studied by NMR metabonomics of plasma samples, **J.Proteome Res.**, 2011 (IF 5.460) In Press
662. Bertini, I., Emsley, L., Felli, I. C., Laage, S., Lesage, A., Lewandoski, D. A., Marchetti, A., Pierattelli, R., and Pintacuda, G., High-Resolution and sensitivity through-bond correlations in ultra-fast MAS solid-state NMR, **Chem.Sci.**, 2, 345-348, 2011
663. Bertini, I., Luchinat, C., Parigi, G., Ravera, E., Reif, B., and Turano, P., Solid-state NMR of proteins sedimented by ultracentrifugation, **Proc.Natl.Acad.Sci.USA**, 108, 10396-10399, 2011 (IF 9.771).
664. Bertini, I., Chevance, S., Del Conte, R., Lalli, D., and Turano, P., The anti-apoptotic Bcl-xL protein, a new piece in the puzzle of cytochrome c interactome, **Plos ONE**, 6, e18329-, 2011 (IF 4.411).
665. Bertini, I., Luchinat, C., and Parigi, G., Moving the frontiers in solution solid state bioNMR. A celebration of Harry Gray's 75th birthday, **Coord.Chem.Rev.**, 255, 649-663, 2011 (IF 10.018).
666. Bertini, I., Banci, L., Cavallaro, G., and Ciofi-Baffoni, S., Seeking the determinants of the elusive functions of Sco proteins, **FEBS J.**, 278, 2244-2262, 2011 (IF 3.129).
667. Bertini, I., Felli, I. C., Gonnelli, L., Vasantha Kumar, M. V., and Pierattelli, R., High-resolution characterization of intrinsic disorder in proteins, **ChemBioChem**, 2011 (IF 3.945) In Press
668. Bertini, I., Gonnelli, L., Luchinat, C., Mao, J., and Nesi, A., A new structural model Aβ40 fibrils, **J.Am.Chem.Soc.**, epub ahead of print, 2011 (IF 9.019).
669. Bertini, I., Case, D. A., Ferella, L., Giachetti, A., and Rosato, A., A grid-enable web portal for NMR structure refinement with AMBER, **Bioinformatics**, 27, 2384-2390, 2011 (IF 4.877).
670. Bertini, I., Cavallaro, G., and Rosato, A., Principles and patterns in the interaction between mono-heme cytochrome c and its partners in electron transfer processes, **Metallomics**, 3, 354-362, 2011 (IF 3.592).
671. Bertini, I., Felli, I. C., Gonnelli, L., Vasantha Kumar, M. V., and Pierattelli, R., ¹³C direct-detection biomolecular NMR spectroscopy in living cells, **Angew.Chem.Int.Ed.**, 50, 1-4, 2011 (IF 12.703).
672. Corzilius, B., Smith, A. A., Barnes, A. B., Luchinat, C., Bertini, I., and Griffin, R. G., High-field dynamic nuclear polarization with high spin transition metal ions, **J.Am.Chem.Soc.**, 133, 5648-5651, 2011 (IF 9.019).

673. Decaria, L., Bertini, I., and Williams, R. J., Copper proteomes, phylogenetics and evolution, **Metalloomics**, 3, 56-60, 2011 (IF 3.592).
674. Oakman, C., Tenori, L., Claudino, W. M., Cappadona, S., Nepi, S., Battaglia, A., Bernini, P., Zafarana, E., Saccenti, E., Fornier, M., Morris, P. G., Biganzoli, L., Luchinat, C., Bertini, I., and Di Leo, A., Identification of a serum-detectable metabolomic fingerprint potentially correlated with the presence of micrometastatic disease in early breast cancer patients at varying risks of disease relapse by traditional prognostic methods, **Ann.Oncol.**, 22, 1295-1301, 2011 (IF 6.452).
675. Polvani, S., Calamante, M., Foresta, V., Ceni, E., Mordini, A., Quattrone, A., D'Amico, M., Luchinat, C., Bertini, I., and Galli, A., Acycloguanosyl 5'-thymidyltriphosphate, a new thymidine analogue prodrug activated by telomerase, reduces pancreatic tumor growth in mice, **Gastroenterology**, 140, 709-720, 2011 (IF 12.403).