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Ivano Bertini

Brief Biography

Ivano Bertini was born on December 6, 1940 in Pisa, Italy. He obtained the Italian degree of Doctor of Chemistry at the University of Florence in 1964 and the Libera Docenza in 1969. He became Full Professor of General and Inorganic Chemistry in 1975 at the University of Florence, where he is to this day. He received the Laurea Honoris Causa from the University of Stockholm in 1998, Ioannina in 2002 and Siena in 2003. He is a member of the Academia Europaea and the Italian Accademia dei Lincei, and is or has been on the editorial staff or advisory board of over 20 of the most authoritative journals in chemistry, biochemistry and inorganic chemistry.

After beginning his research in theoretical/physical inorganic chemistry, since 1975 he has studied the structure-function relationship of metalloproteins through biophysical methods. In 1990, he transformed his lab into an NMR lab for structural biology of metalloproteins, and eventually pioneered the exploitation of genome data banks. He has pursued advancements in technology for solution structure determination, particularly for paramagnetic metalloproteins, and developed specific software applications. He has studied electron and nuclear relaxation from both experimental and theoretical points of view. He has also established a molecular biology department for high-throughput protein expression in structural genomics projects on metalloproteins. Recently he has begun browsing genomes for pharmaceutical targets. He has published over 600 research articles and has solved more than 100 protein structures.

In 1999 he founded the present Center of Magnetic Resonance (CERM) at the University of Florence in an independent and prestigious building hosting an impressive battery of NMR spectrometers. The Center constitutes a major NMR infrastructure in the Life Sciences. Flanking laboratories and spin-off institutions have flourished around CERM in the fields of biotechnology and drug discovery thanks to his leadership.

Degree

Doctorate in Chemistry, 110/100 cum laude, July 1964, University of Florence, Italy
Libero Docente, October 1969

Positions Held

(All at the University of Florence)
Voluntary Assistant 1964-1973
Research Assistantship (Fellowship) CNR (National Research Council - Italy) 1964-1965
Lecturer Chemistry I Laboratory 1965-66
Lecturer Advanced Inorganic Chemistry 1966-68
Lecturer in Chemistry (Faculty of Engineering) 1967-68
Lecturer in Advanced Inorganic Chemistry 1969-76
Full Professor of General and Inorganic Chemistry (Faculty of Pharmacy) 1975-81
Full Professor of General and Inorganic Chemistry (Faculty of Science) 1981-

Visits

Visiting researcher, ETH, Zurich, Switzerland, 1965
Research Associate at Princeton University, N.J., USA, 1968-69
NATO Senior Scientist, California Institute of Technology, USA, 1974
Visiting Professor, University of California at Los Angeles, USA, 1982
CNR Visiting Professor, University of Frankfurt, Germany, 1989
Visiting Professor, University of Strasbourg, France, 1992 and 1993

Visiting scientist, California Institute of Technology, USA, 1995
Visiting scientist, Medical Research Center, University of Cambridge, UK, 1998
Visiting Professor, University of Ioannina, Greece, 1998
Visiting Professor, University of Utrecht, The Netherlands, 2001
Visiting Professor, Chalmers University of Technology, Göteborg, Sweden 2004

Honors

Laurea Honoris Causa in Chemistry, University of Stockholm, Sweden, 1998
Laurea Honoris Causa in Chemistry, University of Ioannina, Greece, 2002
Laurea Honoris Causa in Biological Sciences, University of Siena, Italy, 2003

Chugaev Diploma of Kurnakov Institute of the Academy of Science, URSS, 1981
Japanese Society for the Promotion of Science, Fellow, Japan, 1985, 1995, 2003
Dedication of an international meeting on "Frontiers of the Chemistry of Metal Ions Approaching the Year 2000", Florence, Italy, 1990 on the occasion of his 50th birthday
Golden Medal of the Magnetic Resonance Group of the Italian Chemical Society, Italy, 1991
Prize Accademia dei Lincei, Italy, 1993
European support of his laboratory as a Large Scale Facility, 1994-2004 and 2006-
Member of the Academia Europaea--London, UK, 1994-
Bijvoet Medal, Utrecht, NL, 1998
Special volumes 272, 273, 275 and 276 of *Inorganica Chimica Acta* for a total of 1271 pages were dedicated to him in 1998.
Sapio NMR Prize, Italy, 1999
Member of the Accademia Nazionale dei Lincei, 2000
IUPAC Fellow 2005
Basolo Medal, Northwestern University, IL, USA 2006
Cannizzaro Medal of the Italian Chemical Society, Florence 2006

Special Lectures

Opening Lecture of the Academic Year at the University of Florence, Italy, 1993
Ziegler-Natta lecturer in Germany 1996, (TU Berlin, Halle, Muenster)
A.D. Little Lecturer at MIT, Cambridge, MS, USA, 1997
E.L. Mütterties Lecturer at Berkeley, CA, USA, 1997
J.M. Bijvoet Lecturer, University of Utrecht, NL 1998
Sapio Prize Lecturer, Biopark, Turin, Italy, 1999
FECS lecturer, Athens 2002

Society Memberships

Italian Chemical Society
American Chemical Society
Society of Biological Inorganic Chemistry

Involvement in Scientific Journals (Board Membership)

JBIC (Journal of Biological Inorganic Chemistry), Founder and Chief Editor 1996-1999, Founding Editor 2000-
European Journal of Inorganic Chemistry, Founder and Editor 1998-1999, Senior Editor 1999-
Accounts of Chemical Research, 1998-1999, Consulting Editor 2000-
Advances in Inorganic Chemistry, 1992-
ChemTracs, Inorganic Chemistry, 1995-

Magnetic Resonance in Chemistry, 1996-
Topics in Bioinorganic Chemistry, 1997-
European Journal of Biochemistry, 1998-
La Chimica e l'Industria, (Chief Editor 1994-95 and Board Member 1996-)
Russian Journal of Coordination Chemistry, 1999-
ChemBioChem. 2000-
Journal of Magnetic Resonance 2003-
Chemistry and Biodiversity 2003-
Chem. Med. Chem. 2006-
Comments in Inorganic Chemistry, 1989-2003

Past Duties:

Gazzetta Chimica Italiana, 1985-1990;
Journal of Inorganic Biochemistry, 1992-1996.
Chemical Speciation and Bioavailability, 1989-1999
Inorganica Chimica Acta, 1975-2003

Editorial Activities

Coeditor with R.S. Drago of "ESR and NMR of Paramagnetic Species in Biological Systems", Reidel, Dordrecht, 1980;
Coeditor with A. Dei and L. Lunazzi of "Advances in Solution Chemistry", Plenum Press, New York, 1981;
Guest editor of Volume 43 of Coordination Chemistry Reviews, special issue, 1982;
Coeditor with R.S. Drago and C. Luchinat of "Coordination Chemistry of Metalloenzymes", Reidel, Dordrecht, 1983;
Coeditor with C. Luchinat, W. Maret and M. Zeppezauer of "Zinc Enzymes", Birkhauser, Basel, 1986;
Coeditor with H.B. Gray of the Series "Progress in Inorganic Biochemistry and Biophysics", Birkhauser, Boston, 1986-1988;
Coeditor with H. Molinari and N. Niccolai of "NMR and Biomolecular Structure", VCH, Weinheim, 1990;
Guest editor of Vol. 120 of Coordination Chemistry Reviews, special issue, 1992;
Guest editor of Magnetic Resonance in Chemistry, special issue on "NMR in Bioinorganic Chemistry", Vol. 31, John Wiley and Sons, Chichester, 1993;
Coeditor with Harry B. Gray, S. Lippard and J.S. Valentine of the book "Bioinorganic Chemistry", University Science Books, Mill Valley, CA, 1994;
Guest Editor of Coordination Chemistry Reviews Elsevier S.A., Volumes 185/186 (May, 1999; 838 pages) and 190/192 (October, 1999; 1285 pages), together with Maurizio Peruzzini, CNR, Italy.
Coeditor with H. Sigel and A. Sigel of the "Handbook on Metalloproteins", Marcel Dekker, Inc.; Basel, Switzerland, 2001
Coeditor with C. Luchinat, G. Parigi, Solution NMR of Paramagnetic Molecules, Elsevier, Amsterdam (2001).
Guest editor of Accounts of Chemical Research, special volume on Structural Genomics, 2003
Coeditor with R. van Eldik of the volume of the Advances in Inorganic Chemistry "Relaxometry of Water-Metal Ion Interaction", vol. 57, Academic Press, The Netherlands 2005.
Coeditor with Gray, H.B.; Stiefel, E.I., Valentine, J.S.; of the "Biological Inorganic Chemistry: Structure & Reactivity", University Science Books, Mill Valley, CA, USA 2006
Coeditor with L. Caglioti, G. Faita, D. Giusto and R. Ugo of the "Encyclopedia of Chemistry" (in Italian), ISEDI, Milan, 1977

Offices Held

Member of the Secretariat of the Italian Association of Inorganic Chemistry from 1973 to 1985 except for 77--78; President of the same Association 81-83.

Elected member of the Administration Council of the University of Florence, 1982-1987 and 2000.

President of the Division of Inorganic Chemistry of the Italian Chemical Society 1987--1990;

Vice president 1990-92; President elect 1992, President 1993-95 and Past President 1996-1999 of the Italian Chemical Society.

Member of the Council of the European Environmental Research Organization 1990-1996.

Member of a Steering Committee of the European Science Foundation on the Chemistry of Metals in Biological Systems, 1990-1997.

Member of the Advisory Panel for the Priority Area on High Technology of NATO, 1993-98 and of Life Sciences and Technology 1999.

Acting Director of "Centro Linguistico d'Ateneo" of the University of Florence, 1996-1998

President of the Fondazione Luigi Sacconi, 1997-

Director of the Interuniversity Consortium of Magnetic Resonance on Paramagnetic Metalloproteins (CIRMMP) 1994- (Recognized by the Italian Government since 1997)

Chair of the PhD programs in chemistry, 1997-2000

Chair of the Diploma programs in chemistry, 1997-2001

Member of the consortium with industrial partners "Masaccio ricerche" 1998-

Member of the consortium with industrial partners "NMR - Biovaccini" 1998-2001

Member of the Council of the National Institute "Biosystems and Biostructures", 1998-

Coordinator of the Concerted Action of the European Commission on NMR in Life Science, 1998-2000 .

Italian representative of the "Fine Analysis of Matter Expert Group", 2000-2001

Coordinator of the International Cooperation Network "NMR Structural Biology in Life Sciences in the Post-Genomic Era", 2000-2004

Director of the Center of Magnetic Resonance (CERM) of the University of Florence, 2000-

Comité d'Evaluation du Lab. de Chimie de Coordination (LCC) Toulouse, France CNRS- 2001

Co-founder and chair of the Scientific Advisory Board of the no profit organization Fondazione Farmacogenomica Fiorgen 2003-

Co-founder and chair Scientific Advisory Board of the of the University Spin off company ProtEra 2003-

Member of Working Group ESFRI on Research Infrastructure for Biology and Medical Science 2004-

Chair of the Working Party on Chemistry in Life Sciences of European Chemical Societies EUCHEMS, 2004 and then

Founder and chair of the Division of Chemistry in Life Sciences of EuCheMS, 2006-

Publications

He is the author of more than 600 publications, written in English, in scientific journals of international reknown (see enclosed list).

Together with C. Luchinat, he is the author of the books: NMR of Paramagnetic Molecules in Biological Systems, Benjamin/Cummings, 1986; and NMR of Paramagnetic Substances, Coord. Chem. Rev. vol. 250, 1996. Together with L. Banci and C. Luchinat, he is co-author of the book: Nuclear and Electron Relaxation, VCH, 1991. In 2001 he published with C. Luchinat and G. Parigi "Solution NMR of paramagnetic molecules. Applications to metallobiomolecules and models", Elsevier.

Together with F. Mani, he is co-author of the following books (in Italian): Basic Chemistry, CEDAM (Padua), 1978, 1981, 1986; Inorganic Chemistry, CEDAM, 1979; Stoichiometry, CEA (Milan), 1972, 1981, 1997. Together with C. Luchinat and A. Rosato he is author of the book Principles of Chemistry at the Computer, Sorbona, (Milano) 1995. Together with C. Luchinat

and F. Mani he is author of the book "Chimica", CEA Milano 2004.

In addition, he is the author of articles published in scientific encyclopedias and articles which popularize science. He is editor of special reports like "Chemicals in Agriculture", 1990, "Depollution planning of the Mediterranean Sea", 1992, "Lo stato della ricerca chimica italiana", 1991 and "La protezione dell'ambiente in Italia" 1995, all published by the Italian Chemical Society.

Conferences

He has been invited to hold conferences at the following *international meetings*:

Symposium on Molecular Spectroscopy, Wroclaw (Poland), 1972; XII European Congress of Molecular Spectroscopy, Wroclaw (Poland), 1977; VII International Conference on Coordination Chemistry, Smolenice (Czechoslovakia), 1978; International Symposium on Electron Spin Resonance, Thessaloniki (Greece), 1979; 11th Annual International Conference on ESR of Inorganic and Biological Systems, Leicester, (UK), 1979; Euchem Conference, Venice (Italy), 1979; Third EUCHEM Conference on Organometallic Chemistry, Trieste (Italy), 1980; IX National Conference on Molecular Spectroscopy with International Participation, Albenga (Bulgaria), 1980; 183rd Meeting of the American Chemical Society, New York (USA), 1981; 15th Annual International Conference: Electron Spin Resonance of Inorganic Radicals and Metal Ions in Inorganic and Biological Systems, Cardiff (UK), 1983; XXIII International Conference on Coordination Chemistry, Boulder, Colorado (USA), 1984; International Symposium on Rare Earth Spectroscopy, Wroclaw (Poland), 1984; Meeting on Supramolecular Chemistry: Biological and Chemical Aspects, Rome (Italy), 1984; International Symposium on Structure and Dynamics of Nucleic Acids, Proteins and Membranes, Rome, 1984; 2nd International Conference on Bioinorganic Chemistry, Algarve (Portugal), 1985; 190th American Chemical Society Meeting, Miami, Flo. (USA), 1985; NATO Workshop on Activation of Small Molecules, Leiden (The Netherlands), 1985; NATO School on Activation of Carbon Dioxide, Bari, 1986; Workshop on Synchrotron Radiation, Frascati, 1986; XXIII Workshop on Coordination Chemistry, Smolenice, (Czechoslovakia) 1987; 194th Meeting of The American Chemical Society, New Orleans, (USA) 1987; XXV International Conference on Coordination Chemistry, Nanjing, (China), 1987; 9th Engineering Foundation Conference on Enzyme Engineering, Santa Barbara, CA (USA) 1987; International Symposium on Molecular and Dynamic Approaches to Electrolyte Solutions, Tokyo, (Japan), 1988; National Workshop on Magnetic Resonance, Fuzhou, (China), 1988; Workshop on NMR of Proteins, Oiso, (Japan) 1989; The Manziana Meetings on Copper Proteins, Manziana 1978, 1984, 1990; The Greek-Italian meeting on Biomolecules, Loutrakis, (Greece) 1990; The French-German-English meeting in Bioinorganic Chemistry, Bodensee, (Switzerland) 1990; Okazaki Conference, (Japan) 1990; XXVIII International Conference on Coordination Chemistry, Gera, (East Germany), 1990; 2nd Eurasia Conference on Chemistry, Seoul (Korea), 1990; 1st International Symposium On Applied Bioinorganic Chemistry, Wuhan, (China), 1990; National meeting on Magnetic Resonance, Kazan, (Soviet Union), 1991; Nato School on the Structure of Surfaces and Clusters, Calabria 1991; National Congress of the French Chemical Society, Strasbourg, (France) 1991; 2nd Italian-Portuguese-Spanish meeting, Albufeira, (Portugal) 1992; 2nd Italian-Israelian meeting, Siena 1992; Trace Elements in Chemistry and Medicine, Loutrakis, (Greece) 1992; 1st EUROBIC Conference on Metal Ions in Biological Systems, Newcastle upon Tyne (UK) 1992; XV Conference on Magnetic Resonance in Biological Systems, Jerusalem, (Israel) 1992; XXI European Conference on Molecular Spectroscopy, Wien (Austria) 1992; 2nd International Symposium on Applied Bioinorganic Chemistry, Canton, (China) 1992; Workshop on Magnetic Spectroscopy on Bioinorganic Transition Metal Centers, Homburg, (Germany) 1993; NATO ASI on Magnetic Resonance and Protein Dynamics, Erice, (Italia) 1993; 10th Conference on Catalysis, Florida (USA) 1993; NATO ASI on NMR of Biological Macromolecules, Kolimbari (Greece), 1993; Gordon Research Conference in Inorganic Chemistry, New Hampshire (USA), 1993; 25th Southeastern Magnetic Resonance Conferences, Gainesville,(USA) 1993; Florida Environmental Conference, Palm Coast, Florida,(USA) 1993; Meeting of the American Chemical Society, San Diego,(USA) 1994; 1st European Conference on "The use of stable isotopes in NMR studies of protein structure, dynamics and function", Paris, (France) 1994; NATO Advanced Research Workshop on "Nuclear Magnetic Resonance of Paramagnetic Macromolecules", Sintra, (Portugal) 1994; NATO Advanced Study Institute, Bioinorganic Chemistry: An Inorganic Perspective of Life, Ixia, Rhodes Island, (Greece) 1994; XXX International Conference on Coordination Chemistry, Kyoto, (Japan) 1994; XVI International Conference on Magnetic Resonance in Biological Systems, Veldhoven, (The Netherlands) 1994; Third International Symposium on applied Bioinorganic Chemistry, Perth, Western Australia, (Australia) 1994; 4th Eurasia Conference on

Chemical Sciences, Kuala Lumpur, Malaysia, 1994; Gordon Conference on Metals in Biology, Ventura, CA, 1995, 2002; ESF meeting on Structures and Dynamics of Biomolecules, Wilbad, (Germany) 1995; Italy-Greece-Portugal-Spain Meeting, Senigallia 1995; Meeting of the Italian Chemical Society, Biological Systems, Castiglione d'Orcia (Siena), 1995; XXV EMBO Meeting, Structure and Function of Proteins, Heidelberg, 1995; VII ICBIC, Lübeck, 1995; International Conference on Application of the Mössbauer Effect, Rimini, 1995; Pacificchem 95, Honolulu, 1995; 2nd European Conference on the use of stable isotopes in NMR, Frankfurt, 1996; Royal Society meeting on NMR of Proteins, Leicester, UK, 1996; Joint IBDG/SBIC meeting on Metal Homeostasis/Metals in Biology, Louvain-la-Neuve, Belgium, 1996; XV Meeting of the Portuguese Chemical Society, Porto, Portugal, 1996; Biodegradation of Organic Pollutants, Mallorca, 1996; EUROBIC 3, The Netherlands 1996; XVII International Conference on Magnetic Resonance in Biological Systems, Keystone, USA, 1996; Gordon Conference on Magnetic Resonance in Biology and Medicine, Ventura, USA, 1997; NATO ARW Molecular Modeling and Dynamics of Biological Molecules Containing Metal Ions, San Miniato, Pisa, Italy, 1997; 4th International Symposium on Applied Bioinorganic Chemistry, Cape Town, South Africa, 1997; ACS meeting in San Francisco, USA, 1997; First Joint Meeting Italian and German Biophysical Societies, Hünfeld, Germany, 1997; NATO/ESF Workshop on Biological Electron-Transfer Chains; Tomar, Portugal 1997; European Biophysical Societies Association meeting 97, Orleans, France 1997; VIII ICBIC Yokohama, Japan, 1997; XXXII International Conference on Coordination Chemistry, Santiago, Chile, 1997; 4th FGIPS Meeting in Inorganic Chemistry, Corfu, Greece, 1997; Fourth Bijvoet Tutorial Symposium, Utrecht, The Netherlands 1998; 3rd European NMR Conference, Oxford, UK 1998; Gordon Conference on Chemical Oceanography, Il Ciocco, Italy 1998; 1st International Conference of the South-East European Countries, Thessaloniki, Greece 1998; Croatia Italian Slovenia Chem, Trieste, 1998; XVIII International Conference on Magnetic Resonance in Biological Systems, Tokyo, Japan 1998; NATO-ASI on Metal-Ligand Interactions in Chemistry, Physics and Biology, Cetraro 1998; The Italian-Swedish Symposium on NMR of Paramagnetic Proteins and Model Systems, Stockholm, Sweden 1998; Italian-Korean Meeting of Inorganic Chemistry (CNR-KOSEF), Seoul, Korea 1998; Workshop on Chemistry of Metals in Medicine, The Industrial Perspective COST Action D8, Ivrea, Italy 1998; NATO ASI on Structural Biology and Magnetic Resonance, Erice, Italy 1999; V International Symposium on applied Bioinorganic Chemistry, Corfu, Greece 1999; ESF Conference on NMR in Molecular Biology, Granada, Spain 1999; 26th International Conference on Solution Chemistry, Fukuoka, Japan 1999; Research Center for Materials Science International Symposium, Nagoya, Japan 1999; 37th IUPAC congress, Berlin Germany 1999; 2nd Copper meeting, Ravello, Italy 1999; Trends in transition metal chemistry: towards the third millennium, Pisa, Italy, 2000; National Symposium on Magnetic Resonance and Biomolecular Structure and Function, Mumbai, India 2000; 41th ENC Experimental Nuclear Magnetic Resonance Conference Asilomar, CA (USA) 2000; Post Eurasia Symposium, Bangkok 2000; First International Conference on Porphyrins and Phthalocyanines, Dijon, France 2000; 34th International Conference on Coordination Chemistry, Edinburgh, Scotland 2000; 5th European Biological Inorganic Chemistry Conference, Toulouse, France, 2000; II Acis-chem Meeting Brijuni, Croatia, 2000; 22nd Discussion Meeting of the GDCh-Division "Magnetische Resonanzspektroskopie", Regensburg, Germany, 2000; International Conference on Structural Genomics 2000, Yokohama, Japan; Keystone Symposium on Frontiers of NMR in Molecular Biology, Montana, USA 2001; Second International Structural Genomics Meeting, Airlie, Virginia, USA 2001; XXVII meeting of the Federation of European Biochemical Societies, Lisbon 2001, Portugal; XIV Conference of the International Society of Magnetic Resonance, Rhodes, Greece 2001; Coping with copper, Roma, 2001; Dechema Conference on Structural Genomics, Frankfurt 2001; Gordon Research Conference on Protein Folding and Dynamics Ventura, CA, USA 2002; Gordon Research Conference on Metals in Biology, Ventura, USA, 2002; NMR: a tool for biology V, Paris, France, 2002; From Genes to Molecules, Certosa di Pontignano, Siena, 2002; Complementary Methods in Structural Biology workshop (CMSB) Grenoble, France, 2002; 7th Eurasia Conference on Chemical Sciences, Karachi, Pakistan 2002; An International NMR Symposium, Tokyo, Japan, 2002; The Danish NMR symposium, Copenhagen, Denmark 2002; 8th FECS conference on Chemistry and the Environment, Athens, Greece 2002; 9th Annual Symposia NMRS, Bangalore, India 2003; 7th International Symposium on Applied Bioinorganic Chemistry, Guanajuato, Mexico 2003, Summer School on Biomolecular Structure and Dynamics, Otočec, Slovenia 2003; II Santa Maria Workshop on Chemistry, Havana, Cuba 2003; Symposium on Biological Inorganic and Related Chemistry, Okazaki, Japan 2003; NMR in molecular Biology, Obernai, France 2003; 2nd International Conference on Chemistry and Its Applications, Doha, Qatar 2003; NMR: a tool for biology VI, Paris, France 2004; 8th Symposium on Applied Bioinorganic Chemistry (ISABC8) Hong Kong 2004; International Symposium on Pharmaceutical and Biomedical

Analysis, Florence 2004; Third International Conference on Porphyrins and Phthalocyanines, New Orleans, LA (USA) 2004; New Theoretical and Spectroscopical Approaches to Inorganic Chemistry Problems, San Feliu de Guixols, Spain 2004; 6th Central European NMR Symposium, Linz Austria 2004, International Conference on Structural Genomics, Washington DC (USA) 2004; ICMRBS XXI, Hyderabad, India 2005, 8th FIGIPAS, Athens, Greece 2005, XXII ICBIC, Ann Arbor, (USA) 2005; ACS meeting, Atlanta, GA (USA) 2006, Forty years of NMR in biological systems, Bethesda, MD (USA) 2006; Frontiers of Biomolecular NMR, Ljubljana, Slovenia 2006, International Conference on Porphyrins and Phthalocyanines Rome, Italy 2006, 47th ENC, Pacific Grove, CA (USA) 2006, Photobiology and Phototherapeutic techniques. Oxidative reactions, damages and therapeutic effects, Montecatini, Italy, 2006; XXII ICMRBS Goettingen, Germany 2006, VIII Central European NMR symposium Debrecen, Hungary 2006.

He has held conferences in the following institutes abroad:

California Institute of Technology, Pasadena, (USA) 1974, 1986, 1994 and 1995; University of Illinois, Urbana, (USA) 1974; University of California, Los Angeles, (USA) 1977, 1982 and 1995; MIT, Cambridge, (USA) 1977, 1993, 1997; University of Pennsylvania, Philadelphia, (USA) 1977 and 1991; Pennsylvania State University, (USA) 1977; Los Alamos Laboratories, New Mexico, 1977; University of Goteborg, University of Umea; University of Uppsala (Sweden), 1978; University of Louvain--La--Neuve, (Belgium) 1979; University of Zurich, Bern, Basel and Fribourg, (Switzerland) 1981, ETH Zurich, (Switzerland) 1982, 1996; University of California at Riverside; California State University at North Ridge, University of California at S. Barbara (USA) 1982; University of Saarland, Saarbrucken, (West Germany) 1983; University of Harvard, (USA) 1984 and 1985; Weitzman Institute, Rehovot, University of Tel--Aviv, Haifa Polytechnic, University of Jerusalem (Israel) 1984; University of Florida, Gainesville, (USA) 1985, 1993; University of Innsbruck, (Austria) 1985 and 1987; University of Nagoya, Kanazawa, Sendai, Tokyo, Osaka, Hakata, Fukuoka, Nagasaki 1985; Institut of Molecular Sciences, Okazaki, (Japan) 1985, 1989 and 2003; Chinese Academy of Sciences, Beijing, (Peoples Republic of China) 1985; Chemical Society Zurich, and University of Basel (Switzerland) 1986; Scripps Clinic, San Diego (USA) 1987; University of California at San Francisco, (USA) 1987, 1996; Thsing Hua University, Beijing and Laboratory of Structural Chemistry of Academia Sinica, Fuhzou, (China), 1988; Duke University, N.C. (USA) 1988; Society for Biotechnologic Research, Braunschweig, (Germany), 1989; University of Valencia 1989; University of Paris at Orsay, (France), 1990; University of Kyoto, (Japan), 1990; Princeton University, Northwestern University at Evanston, (USA), 1991, 2000; University of Lund, (Sweden), 1991; University of Beersheva, (Israel), 1991; University of Thessaloniki, (Greece) 1992, University of Michigan, Madison (USA) 1993, Amherst College, Massachusetts, 1993; University of Freiburg, (Germany), 1994; Berlin, Schering 1994; Italian Embassy in London, 1994; University of Brighton, 1994; University of Ohio at Columbus, 1994; J. W. Goethe University, Frankfurt, (Germany), 1995; Technical University and University of Copenhagen, (Denmark) 1995; Waseda University, Tokyo (Japan) 1995; Technical University, Berlin, University of Halle and University of Munster, (Germany) 1996; Columbia University, New York (USA) 1996; John Hopkins University, Baltimore (USA) 1996; University of Munich, (Germany) 1996, University of California at Berkley, (USA) 1997; University of La Laguna, Tenerife, Spain (1997); University of Ioannina, (Greece) 1998; University of Liege (Belgium), 1999; University Marie Curie Paris VI, Paris, (France) 1999, University of Utrecht, (The Netherlands) 2001; Max-Planck Institute, Goettingen 2002 (Germany); EMBL, Heidelberg (Germany) 2002; Forschungsinstitut fuer Molekulare Pharmakologie NMR, Berlin, (Germany) 2004, University of Patras, (Greece) 2004; University of Ioannina, (Greece) 2004; Columbia University, New York, USA 2005, Medical Center Research Institute, Scarborough, ME, USA 2005; University of Evry, Evry, (France) 2005; Northwestern University, Evanston, IL, USA 2006.

He has been invited to hold conferences at the following Italian Institutes:

University of Perugia 1972; University of Cagliari 1974; University of Padua 1974, 1988 and 1989; University of Milan 1975, 1992-; University of Naples 1978; University of Parma 1979, 1983, 1986 1997 and 2000; University of Modena 1980, 1985, and 1998; Italian Meeting on the Chemistry of Living Systems, Modena 1986; University of Catania, 1986, 1993, 2000; University of Ferrara 1987; University of Trieste, 1987, University of Siena 1988; University of Calabria 1990; Sicilian meeting of the Chemical Society, Milazzo 1991; Sacconi's memorial lecture, Cagliari 1993; Opening of the Accademy Year, University of Florence, 1993; CNR

Research Area, Milano 1994; Meeting of the Division of Inorganic Chemistry, Bressanone, 1994; Gruppo di Discussione di Risonanze Magnetiche, Verona, 1995; International School for Advanced Studies, Trieste 1995; University of Turin, 1997; University of Udine, 1997; Biopark of the University of Turin, Ivrea 1999; IV School of Inorganic Chemistry, Lecce, 1999; Istituto Nazionale Biosistemi e Biovaccini, Roma, 2000, Accademia Nazionale dei Lincei, Roma, 2001, 2006; University of Bologna 2001; University of Sassari, 2001; University of Ferrara 2002; Meeting of the Italian Chemical Society, Modena, 2002; University of Siena 2004, Accademia Nazionale Dei Lincei, 2006.

Organization of Congresses

He has been quiet active un the organization of the scientific events in order to promote the branches of science of interest and to acquire new vision and technologies.

Together with Harry B. Gray (California Institute of Technology), Malmström B. G. (Göteborg University) and H. Sigel (University of Basel) he has implemented the series of "International Conference on Bioinorganic Chemistry". He has organized the 1st in 1983 and the 10th in 2001. He has been in the International Organizing Committee of all other ICBICS: International Conference of Bioinorganic Chemistry, Second to Eleventh Portugal 1985, Holland 1987, Boston 1989, Oxford 1991, S. Diego 1993; Lübeck, 1995; Yokohama, 1997, Minneapolis 1999, Cairns 2003, Ann Arbour, 2005. He was one of the ? characters in founding the series of Eurobic of which he organized the second edition in 1994. During the European Research Conference on "Chemistry of Metals in Biological Systems" which he organized in San Miniato in 1995 he founded the Society of Biological Inorganic Chemistry and the Journal of Biological Inorganic Chemistry of which he was the founding editor. He organized a series of Swiss-Italian Symposium on Inorganic Chemistry. 1st in Bressanone, 1981 2nd Friburg 1983, 3rd Ferrara 1986, 4th Neuchâtel 1988, 5th Parma 1990. This series eventually merged with the series French-German-English meetings in Bioinorganic Chemistry to give rise to the Eurobic series. The first of the series was held in Newcastle upon Tyne in 1992 with his participation in the International Organizing Committee.

As a researcher in NMR he organized:

NATO School on "EPR and NMR of Paramagnetic Systems of Biological Interest", Tirrenia 1975; NATO School on "EPR and NMR of Inorganic and Bioinorganic Systems", Maratea 1979;

NATO School on "Coordination Chemistry of Metalloenzymes", S. Miniato, 1982.

He founded the series of Chianti Workshop on Magnetic Resonance:

Cochairman with E. Tiezzi of the 1st and 2nd "Chianti Workshop on Magnetic Resonance", S. Miniato 1984 and 1987; Cochairman of the 3rd of the series with J.W. Emsley, Southampton, UK, San Miniato 1989; Cochairman of the 4th of the series with J. Kowalewski, Stockholm, Sweden, San Miniato, 1991; Cochairman of the 5th of the series with G. Bodenhausen, Lausanne, Switzerland, San Miniato, 1993; Cochairman of the 6th of the series with K. Möbius, Berlin, Germany, San Miniato, 1995; Cochairman of the 7th of the series with Z. Luz, Rehovot, Israel, San Miniato 1997; Cochairman of the 8th of the series with D. Canet, Nancy, France, San Miniato 1999; Cochairman of the 9th of the series with B. Halle, Lund, Germany, Tirrenia 2001, Cochairman of the 10th of the series with D. Fushman, College Park, USA; San Miniato 2003. All the Chianti Workshops were organized with the University of Pisa and Siena.

He has also organized:

Inauguration of the Large Scale Facility for Relaxometry and Magnetic Resonance, Florence 1996;

Chairman of the XXXIII International Conference on Coordination Chemistry, Florence 1998;

Inauguration of the NMR center of the University of Florence in the new campus, March 1999;

the 3rd Meeting of the Users of the Large Scale Facilities for NMR in Life Sciences and Meeting of the Concerted Action for NMR in Life Sciences (NMRCONCERT), Viareggio, 1999.

Chairman of the International Conference on Genome-Based Drug Discovery, Florence 2004.

The organization of the XIX International Conference on Magnetic Resonance in Biological Systems, Florence, 2000 is a major event in this field of activity.

For fun he started with Bernd M. Rode (University of Innsbruck) and Hitoshi Ohtaki (Tokyo

Institute of Technology) the series of the Eurasia Conference on Chemistry:

Eurasia 1st to 7th Conference on Chemistry, Bangkok, 1988, Seoul 1990, Bangkok 1992 (chair of the International Organizing Committee), Kuala Lumpur, 1994, Guangzhou, China 1996; Brunei 2000, Karachi, Pakistan 2002, Hanoi 2004, 2006 (chair of the IOC).

At the European level he started a series of meetings on Inorganic Chemistry: Italian-Portuguese-Spanish in Gandia 1990, Albufeira 1992, Senigallia 1995 (with Greece joining the initiative), Corfù 1997 (with French participation). The series will continue. He started the series of the European Conference on Chemistry for Life Sciences, organizing the 1st in Rimini 2005 and inspired the birth of the series of Central European Conference on Chemistry towards Biology (Slovenia 2002).

Cochairman with L. Lunazzi of the "V Symposium on Solute-Solute-Solvent Interactions, Florence 1980;

Symposium on Achievements and Perspectives in Coordination Chemistry in honor of Prof. L. Sacconi, Florence, 1981;

Cochairman with M. Zeppezauer of the "International Workshop on Zinc Enzymes", S. Miniato 1985;

Cochairman with W. Rutter of the Workshop on "Genetic and Physico-Chemical Approaches for the Analysis of Biological Catalysts", Florence 1986 and coorganizer of the Workshop on "Structure and Function of Mutated Proteins", Florence, 1991;

Chairman of the Symposium on Environmental Biotechnology, S. Miniato, 1989;

Cochairman with G. Grassi of the "1st European Forum on Electricity Production from Biomass and Solid Wastes by Advanced Technologies", Florence, 1991;

Workshop on Bioinorganic and Biotechnological Aspects of Environmental Chemistry, Florence 1992;

International Steering Committee of Bioinorganic and Biotechnological Aspects of Environmental Chemistry-2, Florence, 1994;

Cochairman of the Mediterraneanchem, an International Conference on Chemistry and the Mediterranean Sea, Taranto, 1995;

Chairperson of the OECD Global Science Forum Workshop on International Cooperation on Structural Genomics, Florence, 2000;

Organizer of the Workshop on Peroxidases and Cyt P450, Le Bischenberg, France 1992.

Summary of Scientific Activities

He has worked as student and post-doctor (Italian doctor degree, 1964) on the infrared characterization of coordination compounds and linkage isomers. Noticeably he proposed a criterium, which is used even nowadays, to distinguish between nitrogen and chalcogen binding of NCS- and NCSe to metal ions on the basis of vibrational spectroscopy. Then he prepared and characterized coordination compounds with unusual coordination numbers. In particular he contributed to the synthesis and characterization of five coordinated metal complexes which made famous in the world the School of his Maestro Luigi Sacconi. With these results he obtained the Libera Docenza in 1969.

The spectroscopic and theoretical approaches to the investigation of coordination compounds led him more deeply into the NMR characterization of paramagnetic compounds in solution. He spent the year 68/69 in Princeton (NJ) with W.De.W. Horrocks Jr. Since his NMR instrument (a DA-60 Varian) was becoming obsolete, he worked on EPR and optical absorption investigations of single crystals. He extensively used ligand field theory to characterize the electronic levels of coordination compounds. He enjoyed working during these years with his young coworker Dante Gatteschi. At this point he was promoted Full Professor (1975).

He had learned how to handle biological materials during a visit with Harry B. Gray at Caltech in 1974. As full Professor, he started his scientific adventure on biological inorganic chemistry with his coworker Andrea Scozzafava (who essentially remained scientifically close to him until 1999) and the undergraduate student Claudio Luchinat who has remained close to him up to now. For a few years he continued also to cultivate coordination chemistry. As bioinorganic chemist he correctly predicted the coordination number around the zinc ion of the inhibitor derivatives of carbonic anhydrase; he described the derivative with HCO₃⁻ as giving rise to an equilibrium between tetra and pentacoordination, the latter coordination allowing the detachment of the substrate. He proposed a model for the interaction of CO₂ within the active

cavity. The electronic spectra of the cobalt substituted enzyme in the absence of inhibitors, which describe the pH dependent properties of the enzyme, were correctly reported for the first time by him.

In 1978, by working on carbonic anhydrase he entered in touch with S.H. Koenig at IBM Yorktown Heights (NY) and his NMRD approach. He continued to work on carbonic anhydrase until the end of the eighties.

In 1980 he started working on carboxypeptidase. During this work he largely interacted with B.L. Vallee at Harvard (MS). He has experimentally shown the occurrence of several steps in the enzymatic mechanism of carboxypeptidase. Carboxylates of acids, aminoacids and peptides, which are substrates of the enzyme, bind at Arg145 first; then the metal binding site becomes accessible to further ligands including N_3^- and NCO^- . These observations were framed into a general description of the mechanism obtained through MD simulations. His new pupil Lucia Banci had learned how to handle MD simulation from the late Peter Kollman from UCSF. He has inspired several X-ray studies performed within his research group, mainly by Stefano Mangani. His scientific interests included alkaline phosphatase, liver alcohol dehydrogenase and transferrins. Alkaline Phosphatase led him to collaborate with the late J.E. Coleman of Yale (CT), and liver alcohol dehydrogenase with M. Zeppenzauer from Saarbruecken.

The characterization of copper-zinc superoxide dismutase (SOD) started with the studies on the copper(II) properties in 1980 and then continued with the NMR of the copper-cobalt derivative, whose NMR spectrum was made possible by the presence of cobalt, and with the investigation of mutated proteins. The activity and the anion affinities were related to the presence of various residues in the active cavity and to the structure of the ligands around the metal ions. He then started with his pupil Maria Silvia Viezzoli the adventure of protein expression and site directed mutagenesis. The interactions with the company Chiron at Emeryville (CA) and with Bill Rutter and R.A. Hallewell were quite significant. He has obtained the structure of reduced SOD in the solid state and in solution. Since the naturally occurring protein is a dimer, he succeeded through site directed mutagenesis to prepare active monomeric species and to solve their solution and solid state structure. The solution and dynamics of SOD derivatives were well characterized. SOD led him to interact with J.S. Valentine from UCLA. He is now involved in the study of the causes of familial Amyotrophic Lateral Sclerosis caused by SOD mutants.

Iron-sulfur proteins were deeply investigated and the oxidation number of each metal ion determined through 1H NMR. He reported for the first time the complete 1H NMR spectra of reduced two-iron-two sulfur proteins. They contain one iron(III) and one iron(II). He showed that the reducible iron is always one and the same. Finally, he showed that the latter is the one on the surface and that solvation is responsible for its reduction potential. Then he showed that the 1H NMR spectra of oxidized HiPIP (High Potential Iron Sulfur Proteins) could be interpreted by assuming that they contain two iron(III) and two iron at the oxidation state + 2.5. These data were interpreted in a unified picture with Moessbauer spectroscopy. He has contributed to the development of a theoretical model based on the Heisenberg exchange coupling scheme in order to explain these properties as well as those of all Fe-S proteins. He proposed a theoretical model which relates proton shifts and oxidation numbers of the iron ions. Such model has been widely used for many similar proteins.

Since late 1989 he had the 600 MHz (1st in Italy and 30th in the world) and eventually tried to solve the solution structure of paramagnetic metalloproteins. The experience in detecting hyperfine shifted and hyperfine broadened signals, together with the MD expertise available in his lab, led him to solve the tridimensional structure of two HiPIP proteins in solution through NMR in the oxidized and reduced forms as well as of some mutants (1994 and afterwards). Since they are paramagnetic and paramagnetism hampers the NMR determination of proton-proton distances, the solution study is an important achievement also for the technological implications.

He then expressed one ^{13}C , ^{15}N enriched HiPIP for structure refinement. These results allowed him to compare the solution structures of oxidized and reduced forms. The reduced form exists as partially unfolded in presence of 4M guanidinium chloride and its structure and mobility were investigated. He solved the solution structure of a ferredoxin containing two Fe_4S_4 clusters, of one containing a Fe_3S_4 and one Fe_4S_4 cluster, of one containing a Fe_2S_2 cluster, and finally, of a rubredoxin which contains a single iron. He has proposed to use hyperfine nuclear relaxation as further structural restraints.

He initiated in 1990 the structural characterization of paramagnetic heme proteins by

characterizing peroxidases and their mutants. He obtained structural information on lignin peroxidase and manganese peroxidase through 2D ¹H NMR spectra when they represented a pionieristic work, and has proceeded to an extensive assignment of the NMR spectra of the above peroxidases as well as of cytochrome c peroxidases. He has discussed the factors determining the redox properties of these systems. He has characterized the binding sites of substrates in horseradish peroxidase, ligninase and manganese peroxidase and has provided information about the mechanism.

Eventually, he afforded the solution structure of various cytochromes c and their mutants both in their diamagnetic reduced state and in the oxidized paramagnetic state. He has shown that the mutant Ala80Met of yeast Cyt c mutant carries oxygen also because Tyr 67 is able to form a hydrogen bond with the bound oxygen. On this occasion he has developed an algorithm to include pseudo contact shifts for the determination of the solution structures. Eventually, he has developed protocols to include paramagnetism based constraints in the popular Dyana and Explor packages for solution structure determination <http://www.postgenomicnmr.net> as well as in the molecular dynamics package Amber 7. He has afforded the problem of comparing the solution structures of several oxidized and reduced Cytochromes c3, b5 and b562. He then compared the mobility in the ms-μs and ns - ps ranges for a series of cytochromes, both oxidized and reduced, Fe-S proteins and Cu,Zn SOD. After the year 2000 mobility studies are routinely associated to structure determination.

He has developed the NMR techniques for the investigation of paramagnetic compounds and the theory of the unpaired electrons-magnetic nuclei coupling. He has investigated small complexes containing coordinated water molecule(s) and metalloproteins through the measurements of water proton longitudinal relaxation times between 0.01 and 600 MHz. He has proposed general computer programs to extract structural and dynamic parameters from nuclear relaxation studies. Such studies have shed light on the mechanism of electron relaxation in solution and on the nature of electron nucleus coupling. These studies provide the theoretical ground for the development of contrast agents in MRI. Before the end of the 20th century he reshaped his research within a post genomic frame by exploiting the genomic banks with bioinformatic tools. So, he revisited mitochondrial cytochromes c and Fe₂S₂ protein. Then he initiated a program tending at the characterization of the proteins involved in copper trafficking in every organism. He then developed a molecular biology laboratory to express proteins. Besides protein structures, he is attempting to design the protein-protein interaction frame which is needed for cellular processes. As a further consequence he entered the field of drug design.

Then the effect of ionic strength and denaturing agents like guanidinium chloride on the structure and dynamics of a number of proteins were investigated. This opened the field of the characterization of partially folded proteins.

He has published more than 600 articles.

In 1996 the lab was equipped with 800 MHz spectrometer and in 2003 with a 900 MHz. In 2001 and 2004 the 500 MHz and 800 MHz respectively, were equipped with cryoprobes.

He has been invited to many congresses and institutions to present and discuss his results. Many visitors have spent periods of time in Florence, from famous scientists in sabbatical leave to young researchers as students and postdoctors. He has organized many meetings and has started series of meetings.

List of Publications (as of January 2007)

1. Sabatini, A. and Bertini, I., Far-infrared spectra of oxochloro and oxobromo complexes of Nb(V), Mo(V), and W(V), **Inorganic Chemistry**, 4, 204-206, 1965
2. Sabatini, A. and Bertini, I., Infrared spectra of substituted thiocyanate complexes. The effect of the substituent on bond type I, **Inorganic Chemistry**, 4, 1665-1667, 1965
3. Sabatini, A. and Bertini, I., Infrared spectra between 100 and 2500 cm⁻¹ of some complex metal cyanates, thiocyanates, and selenocyanates, **Inorganic Chemistry**, 4, 959-961, 1965
4. Bertini, I. and Sabatini, A., Infrared spectra of substituted thiocyanate complexes. The effect of the substituent on bond type II, **Inorganic Chemistry**, 5, 1025-1028, 1966
5. Sacconi, L. and Bertini, I., High-spin five-coordinated 3d metal complexes with pentadentate Schiff bases, **J.Am.Chem.Soc.**, 88, 5180-5185, 1966
6. Sacconi, L. and Bertini, I., Nickel(II) complexes with N,N'-tetramethylalkylenediamines,

Inorg.Nucl.Chem.Letters, 2, 29-32, 1966

7. Sacconi, L. and Bertini, I., Complexes of copper(II) with Schiff bases formed from salicylaldehydes and N-substituted ethylenediamines, **Inorganic Chemistry**, 5, 1520-1522, 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, **Inorganic Chemistry**, 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, **Inorganic Chemistry**, 6, 2032-2035, 1967

10. Sacconi, L., Bertini, I., and Morassi, R., High-spin five-coordinate nickel(II) and cobalt(II) complexes with a tridentate NNN Schiff base, **Inorganic Chemistry**, 6, 1548-1553, 1967

11. Sacconi, L. and Bertini, I., Five-coordinate nickel(II) complexes with nitrogen-phosphorus and nitrogen-arsenic tetradentate ligands, **J.Am.Chem.Soc.**, 89, 2235-2236, 1967

12. Sacconi, L., Bertini, I., and Mani, F., Metal complexes of N,N,N',N'-tetramethyldiamines. I. Nickel(II) and cobalt(II) complexes, **Inorganic Chemistry**, 6, 262-267, 1967

13. Ciampolini, M. and Bertini, I., A ligand-field model for high-spin five-coordinate complexes of cobalt(II), **Journal of Chemical Society Inorganic Physical and Theoretical**, 2241-2244, 1968

14. 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

15. Sacconi, L. and Bertini, I., Four- and five-coordinated complexes of cobalt(II) and nickel(II) with tridentate Schiff bases, **Inorganic Chemistry**, 7, 1178-1183, 1968

16. Sacconi, L., Bertini, I., and Mani, F., Five-coordination with "hybrid" ligands. II. Nickel(II) complexes with polyfunctional arsenic-containing ligands, **Inorganic Chemistry**, 7, 1417-1420, 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, **Chemical Communication**, 1471-1472, 1969

18. Mani, F. and Bertini, I., Cobalt(II) and nickel(II) complexes with N,N,N'-trimethylated and triethylated alkylenediamines, **Inorganica Chimica Acta**, 3, 451-454, 1969

19. 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, **Inorganica Chimica Acta**, 629-631, 1970

20. Bertini, I. and Mani, F., The existence of five-coordinate high-spin nickel(II) complexes with mixed salicylaldehyde ligands, **Inorganic Chemistry**, 9, 248-251, 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. II. Five-coordinate complexes, **Inorganic Chemistry**, 9, 698-702, 1970

22. 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, **Inorganica Chimica Acta**, 4, 79-80, 1970

23. 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, **Inorganic Chemistry**, 9, 693-698, 1970

24. Wilson, L. J. and Bertini, I., *Cis-trans*-isomerism in solution for the tris-(N-p-tolylpyridinaldimine)cobalt(II) cation, **Chemical Communication**, 1589-1590, 1970

25. Bertini, I., Ciampolini, M., and Sacconi, L., Polarized spectra of the trigonal bipyramidal CoNP₃Br chromophore, **J.Coord.Chem.**, 1, 73-74, 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 $[\text{Ni}(\text{N}_3\text{P})\text{Br}]\text{B}(\text{C}_6\text{H}_5)_4$, **Inorganic Chemistry**, 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, **Journal of Chemical Society Inorganic Physical and Theoretical**, 489-492, 1971
28. Bertini, I. and Gatteschi, D., Polarized single-crystal electronic spectrum of a high-spin NiN_3O_2 chromophore, **J.Coord.Chem.**, 1, 285-288, 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, **Inorganic Chemistry**, 10, 865-868, 1971
30. Wilson, L. J. and Bertini, I., NMR detection of cis and trans isomers of pseudooctahedral 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. and Gatteschi, D., Single crystal polarized spectra of the $\text{Cu}(\text{en})_3\text{SO}_4$ complex, **Inorg.Nucl.Chem.Letters**, 8, 207-210, 1972
33. Bertini, I., Gatteschi, D., and Mani, F., Single-crystal electronic spectra of NiPI_3 chromophore, **Inorganic Chemistry**, 11, 2464-2468, 1972
34. 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, **Inorganic Chemistry**, 11, 1323-1326, 1972
35. Bertini, I., Ciampolini, M., Dapporto, P., and Gatteschi, D., Polarized single-crystal spectrum of a high-spin trigonal- bipyramidal NiN_5 chromophore, **Inorganic Chemistry**, 11, 2254-2258, 1972
36. 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, **Inorganica Chimica Acta**, 6, 185-187, 1972
37. Bertini, I. and Sacconi, L., Proton magnetic resonance spectra of paramagnetic molecules, **J.Mol.Struct.**, 19, 371-385, 1973
38. 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
39. Bertini, I., Gatteschi, D., and Mani, F., Single-crystal polarized electronic spectra of tetra-*n*- butylammonium tribromo(quinoline)cobaltate(II), **Inorganica Chimica Acta**, 717-720, 1973
40. Bertini, I., Ciampolini, M., and Gatteschi, D., Single-crystal polarized electronic spectra of a CoN_5 chromophore, **Inorganic Chemistry**, 12, 693-696, 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, **Inorganic Chemistry**, 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 spectra of bis-*N-t*-butylpyrrol-2- aldiminocopper(II) complexes, **Gazz.Chim.Ital.**, 104, 1029-1032, 1974
44. Bertini, I., Gatteschi, D., and Scozzafava, A., Single crystal ESR study of the $\text{Cu}(\text{en})_3\text{SO}_4$ complex, **Inorganica Chimica Acta**, 11, L17-L19, 1974
45. Bertini, I., Dei, A., and Scozzafava, A., Proton magnetic resonance spectra of bis(N-alkylsalicylaldiminato)copper(II) complexes, **Inorganic Chemistry**, 14, 1526-1528, 1975
46. Bertini, I., Gatteschi, D., Paoletti, P., and Scozzafava, A., A comment on the Jahn-Teller effect in the complex $\text{K}_2\text{PbCu}(\text{NO}_2)_6$, **Inorganica Chimica Acta**, 13, L5-L6, 1975
47. Bertini, I., Gatteschi, D., and Scozzafava, A., Ligand field interpretation of high-spin

- trigonal-bipyramidal cobalt(II) complexes, **Inorganic Chemistry**, 14, 812-815, 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, **Inorganic Chemistry**, 14, 1639-1643, 1975
49. Bertini, I., Gatteschi, D., and Scozzafava, A., Single crystal polarized electronic spectra of the complex bis(N-t-butylpyrrole-2-carbaldimino)cobalt(II), **Inorganica Chimica Acta**, 13, 145-148, 1975
50. Bertini, I., Luchinat, C., and Scozzafava, A., ¹³C NMR spectra of hexakis pyridine-N-oxide cobalt(II) and nickel(II) complexes, **Inorganica Chimica Acta**, 19, 201-202, 1976
51. Bertini, I., Luchinat, C., and Scozzafava, A., Interaction of cobalt bovine carbonic anhydrase with the acetate ion, **Biochim.Biophys.Acta**, 452, 239-244, 1976
52. 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, **Inorganic Chemistry**, 15, 203-207, 1976
53. Bertini, I., Luchinat, C., and Scozzafava, A., Stereochemistry of cobalt(II) in cobalt bovine carbonic anhydrase and its derivatives, **Inorganica Chimica Acta**, 22, L23-L24, 1977
54. 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
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.Comm.**, 78, 158-160, 1977
56. Bertini, I., Gatteschi, D., and Scozzafava, A., Ligand field parameters, **Israel J.Chem.**, 15, 189-199, 1977
57. 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
58. Bertini, I., Gatteschi, D., and Scozzafava, A., Jahn-Teller distortions of tris(ethylenediamine)copper(II) complexes, **Inorganic Chemistry**, 16, 1973-1976, 1977
59. Bertini, I., Luchinat, C., and Scozzafava, A., Interactions between α -Amino acids and cobalt(II) bovine carbonic anhydrase, **Bioinorg.Chem.**, 7, 225-231, 1977
60. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Proton relaxation of water solutions containing copper carbonic anhydrase, **Inorganica Chimica Acta**, 23, L15-L16, 1977
61. Bertini, I., Luchinat, C., and Scozzafava, A., A ³¹P 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., Paramagnetic metal ions as structural probes for NMR investigation of inorganic and bioinorganic compounds, **J.Mol.Struct.**, 45, 173-197, 1978
63. 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
64. 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
65. Bertini, I., Luchinat, C., and Scozzafava, A., Binding affinity of bicarboxylate ions for cobalt(II) bovine carbonic anhydrase, **Bioinorg.Chem.**, 9, 93-100, 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., Borghi, E., and Luchinat, C., Characterization of nickel(II) bovine carbonic anhydrase and its inhibitor derivatives, **Bioinorg.Chem.**, 9, 495-504, 1978
68. 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
69. Barzi, D., Bertini, I., Luchinat, C., and Scozzafava, A., The electronic spectra of cobalt(II) bovine carbonic anhydrase, **Inorganica Chimica 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 bipyramid, **Inorganic Chemistry**, 17, 3194-3197, 1979
71. Bertini, I., Luchinat, C., and Scozzafava, A., ³¹P NMR spectra of paramagnetic MBr₂(OPPh₃)₂ complexes. A breakdown in the validity of the Solomon-Bloembergen equations, **Inorg.Nucl.Chem.Letters**, 15, 89-91, 1979
72. Bertini, I., Canti, G., Kozlowski, H., and Scozzafava, A., Spectroscopic characterization of copper(II) thermolysin, **J.Chem.Soc.Dalton Trans.**, 1270-1273, 1979
73. Bertini, I., Dapporto, P., Gatteschi, D., and Scozzafava, A., Static-dynamic distortions of the tris(1,2-diaminoethane)copper(II) cation [Cu(en)₃]²⁺. Crystal structures of the salts [Cu(en)₃][SO₄] at 120 K and of [Cu(en)₃]Cl₂·0.75 en at 298 K, **J.Chem.Soc.Dalton Trans.**, 1409-1414, 1979
74. Bertini, I., Borghi, E., and Luchinat, C., Investigation of the system CO₂-HCO₃⁻ in the presence of copper(II) bovine carbonic anhydrase B, **J.Am.Chem.Soc.**, 101, 7069-7071, 1979
75. Bertini, I., Gatteschi, D., and Scozzafava, A., Six-coordinate copper complexes with g_z < g_x in the solid state, **Coord.Chem.Rev.**, 29, 67-84, 1979
76. Bertini, I., Canti, G., Luchinat, C., and Scozzafava, A., Characterization of oxovanadium(IV) substituted bovine carbonic anhydrase B, **Inorganica Chimica Acta**, 36, 9-12, 1979
77. 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
78. Bertini, I., Luchinat, C., and Scozzafava, A., Some structural aspects of carbonic anhydrase, in: Biophysics and physiology of carbon dioxide, Bauer, C., Gros, G., and Bartels, H., 151,
79. Bertini, I., Canti, G., Luchinat, C., and Romanelli, P., Cyanometallates and cobalt(II) bovine carbonic anhydrase B. Five coordination with dicyanoaurate(I), **Inorganica Chimica Acta**, 46, 211-214, 1980
80. Bertini, I., Luchinat, C., and Scozzafava, A., The acid-base equilibria of carbonic anhydrase, **Inorganica Chimica Acta**, 46, 85-89, 1980
81. Bertini, I., The electronic ground state of 3d metal ions with respect to the ESR and NMR experiment, in: ESR and NMR of paramagnetic species in biological and related systems, Bertini, I. and Drago, R. S., 201,
82. Bertini, I., Canti, G., Luchinat, C., and Mani, F., The complex cation [Co{tris(3,5-dimethyl-1-pyrazolylmethyl)amine} H₂O]²⁺: a model for metalloenzymes containing bipoisitive zinc(II) chromophores with a water molecule in the coordination sphere, **Inorganica Chimica Acta**, 46, L91-L92, 1980
83. 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, **Inorganic Chemistry**, 19, 2198-2200, 1980
84. Bertini, I., Luchinat, C., Mani, F., and Scozzafava, A., Adducts of bis(N-substituted ethylenediamine)copper(II) complexes with hexacyanoferrate(III), **Inorganic Chemistry**, 19, 1333-1336, 1980
85. 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
86. 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
87. 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

88. Bertini, I. and Scozzafava, A., Copper(II) as probe in substituted metalloproteins, in: Metal ions in biological systems, Sigel, H., 31,
89. Bertini, I., The investigation of coordinated water in paramagnetic metalloproteins through nuclear magnetic resonance spectroscopy, **Comments Inorg.Chem.**, 1, 227-243, 1981
90. Bertini, I., Luchinat, C., and Borghi, E., A fourier-transform NMR investigation of $[(C_4H_9)_4Z][MP(C_6H_5)_3]_3$ (Z = N,P; M = Co,Ni), **Inorganic Chemistry**, 20, 303-306, 1981
91. Bertini, I., Canti, G., and Luchinat, C., ^{17}O NMR investigation of copper(II) substituted carbonic anhydrases, **Inorganica Chimica Acta**, 56, 1-4, 1981
92. 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
93. Bertini, I., Luchinat, C., and Messori, L., A water ^{17}O NMR study of the pH dependent properties of superoxide dismutase, **Biochem.Biophys.Res.Comm.**, 101, 577-583, 1981
94. Bertini, I., Canti, G., and Luchinat, C., Water in the coordination sphere of metalcarbonic anhydrases: a solvent proton longitudinal relaxation study at several frequencies, **Inorganica Chimica Acta**, 56, 99-107, 1981
95. Bertini, I., Canti, G., Luchinat, C., and Mani, F., pH-dependent properties of a $CoN_4(OH_2)$ chromophore: a spectroscopic model of cobalt carbonic anhydrase, **Inorganic Chemistry**, 20, 1670-1673, 1981
96. 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
97. Bertini, I., Canti, G., and Luchinat, C., 1H NMR study of cobalt(II)-substituted carboxypeptidase A, **J.Am.Chem.Soc.**, 104, 4943-4946, 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., Canti, G., Luchinat, C., and Messori, L., 1H NMR detection of $CoOH_2 \leftrightarrow CoOH$ interconversions in high- spin cobalt(II) complexes, **Inorganic Chemistry**, 21, 3426-3429, 1982
100. Bertini, I., Canti, G., and Luchinat, C., Preparation and characterization of the vanadium(III) derivative of transferrin, **Inorganica Chimica Acta**, 67, L21-L23, 1982
101. 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, **Inorganica Chimica Acta**, 67, 99-102, 1982
102. 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
103. Bertini, I., Lanini, G., and Luchinat, C., 1H NMR relaxation rate and coordination number in high spin cobalt(II) complexes, **Inorganica Chimica Acta**, 80, 123-126, 1983
104. Bertini, I., The coordination properties of the active site of zinc enzymes, in: The coordination chemistry of metalloenzymes, Bertini, I., Drago, R. S., and Luchinat, C., 1,
105. Bertini, I. and Luchinat, C., An insight on the active site of zinc enzymes through metal substitution, in: Metal ions in biological systems, Sigel, H., 101,
106. Bertini, I., Luchinat, C., and Scozzafava, A., A comment on anion binding to superoxide dismutase, in: The coordination chemistry of metalloenzymes, Bertini, I., Drago, R. S., and Luchinat, C., 155,
107. Bertini, I., Lanini, G., Luchinat, C., and Monnanni, R., Spectroscopic studies on cobalt(II) carboxypeptidase A, in: The coordination chemistry of metalloenzymes, Bertini, I., Drago, R. S., and Luchinat, C., 93,
108. Bertini, I., Canti, G., Luchinat, C., and Borghi, E., Investigation of the system copper(II) carbonic anhydrase and HCO_3^-/CO_2 , **J.Inorg.Biochem.**, 18, 221-229, 1983

109. Bertini, I., Luchinat, C., Scozzafava, A., Maldotti, A., and Traverso, O., Investigation of the copper-magnesium-alkaline phosphatase system, **Inorganica Chimica Acta**, 78, 19-22, 1983
110. Bertini, I., Lanini, G., and Luchinat, C., Equilibrium species in cobalt(II) carbonic anhydrase, **J.Am.Chem.Soc.**, 105, 5116-5118, 1983
111. 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
112. 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
113. 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 H₂O-models, **Biophys.J.**, 41, 179-187, 1983
114. 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, **Inorganic Chemistry**, 23, 1422-1425, 1984
115. 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?, **Inorganica Chimica Acta**, 91, 173-177, 1984
116. Bertini, I., Luchinat, C., Monnanni, R., Scozzafava, A., and Borghi, E., Investigation of zinc-deprived bovine superoxide dismutase, **Inorganica Chimica Acta**, 91, 109-111, 1984
117. 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
118. 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
119. Bertini, I., Luchinat, C., Messori, L., and Scozzafava, A., Cobalt(II) as an NMR probe for the investigation of the coordination sites of conalbumin, **European Journal of Biochemistry**, 141, 375-378, 1984
120. 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
121. Bertini, I., Lanini, G., and Luchinat, C., ^1H NMR spectra of reduced spinach ferredoxin, **Inorganic Chemistry**, 23, 2729-2730, 1984
122. Bertini, I., Lanini, G., and Luchinat, C., A water ^1H and ^{17}O N.M.R. study on PHG-modified SOD, **Inorganica Chimica Acta**, 93, 51-53, 1984
123. 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
124. 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
125. 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
126. Banci, L., Bertini, I., and Luchinat, C., Solvent ^1H NMRD of copper(II) complexes, **Chem.Phys.Lett.**, 118, 345-347, 1985
127. Banci, L., Bertini, I., and Luchinat, C., ^1H NMRD studies of solutions of paramagnetic metal ions in ethyleneglycol, **Inorganica Chimica Acta**, 100, 173-181, 1985
128. Banci, L., Bertini, I., and Luchinat, C., Lanthanide ions as NMR probes, in: Rare Earths Spectroscopy, Trebiatowska, B. J., Legendziewicz, J., and Streck, W., 80,
129. Bertini, I., Luchinat, C., and Messori, L., Spectral characterization of vanadium-

- transferrin systems, **J.Inorg.Biochem.**, 25, 57-60, 1985
130. 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
131. Bertini, I. and Luchinat, C., High spin cobalt(II) as a probe for the investigation of metalloproteins, **Adv.Inorg.Biochem.**, 6, 71-111, 1985
132. Bertini, I. and Luchinat, C., Metal ions in biochemistry, in: Structure and motion: membranes, nucleic acids and proteins, Clementi, E. and et al., 293,
133. Bertini, I., Lanini, G., Luchinat, C., and Monnanni, R., Investigation of cobalt(II) substituted carboxypeptidase A interacting with azide and cyanate ions, **Inorganica Chimica Acta**, 107, 153-157, 1985
134. Bertini, I., Luchinat, C., Mancini, M., and Spina, G., The dipolar coupling between unpaired electrons and resonating nuclei, in: Magneto-structural correlations in exchange-coupled systems, Gatteschi, D., Kahn, O., and Willett, R. D., 421,
135. 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
136. Bertini, I., Dei, A., Luchinat, C., and Monnanni, R., Acid-base properties of cobalt(II)-substituted carbonic anhydrases, **Inorganic Chemistry**, 24, 301-303, 1985
137. Bertini, I., Lanini, G., Luchinat, C., Messori, L., Monnanni, R., and Scozzafava, A., Investigation of $\text{Cu}_2\text{Co}_2\text{SOD}$ and its anion derivatives. ^1H NMR and electronic spectra, **J.Am.Chem.Soc.**, 107, 4391-4396, 1985
138. 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
139. 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
140. 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
141. Bertini, I., Luchinat, C., and Monnanni, R., Zinc enzymes, **J.Chem.Educ.**, 62, 924-927, 1985
142. 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.Comm.**, 133, 787-793, 1985
143. 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, **Inorganica Chimica Acta**, 107, L21-L22, 1985
144. Banci, L., Bertini, I., and Luchinat, C., Electron relaxation, **Magn.Reson.Rev.**, 11, 1-40, 1986
145. 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
146. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., Scozzafava, A., and Salvato, B., A spectroscopic investigation of Co_2Zn_2 - and Co_2Co_2 - superoxide dismutase, **Gazz.Chim.Ital.**, 116, 51-54, 1986
147. Bertini, I., Dei, A., Luchinat, C., and Monnanni, R., Anion binding properties of cobalt(II)-substituted carbonic anhydrases, in: Zinc enzymes, Bertini, I., Luchinat, C., Maret, W., and Zeppezauer, M., 371,
148. Bertini, I., Luchinat, C., Messori, L., Scozzafava, A., Pellacani, G. C., and Sola, M., ^{13}C NMR study of the synergistic anion in transferrins, **Inorganic Chemistry**, 25, 1782-1786, 1986
149. Bertini, I., Luchinat, C., and Viezzoli, M. S., Metal substitution as a tool for the investigation of zinc proteins, in: Zinc Enzymes, Bertini, I., Luchinat, C., Maret, W., and

Zeppezauer, M., 27,

150. Bertini, I. and Luchinat, C., NMR studies on copper(II) containing biological molecules, in: *Biological and Inorganic Copper Chemistry*, Karlin, K. D. and Zubieta, J., 23,

151. Bertini, I., Briganti, F., and Luchinat, C., Solvent proton nuclear magnetic relaxation dispersion (NMRD) in solutions of paramagnetic macromolecules, in: *Advances in magnetic resonance techniques in systems of high molecular complexity*, Niccolai, N. and Valensin, G., 165,

152. 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. Am. Chem. Soc.**, 47, 1193-1196, 1986

153. 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

154. 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

155. Rosi, M., Sgamellotti, A., Tarantelli, F., Bertini, I., and Luchinat, C., Ab initio calculations of the Cu^{2+} - O_2^- interaction as a model for the mechanism of copper-zinc superoxide dismutase, **Inorganic Chemistry**, 25, 1005-1008, 1986

156. Banci, L., Bertini, I., Luchinat, C., and Scozzafava, A., Nuclear relaxation in the magnetic coupled system $\text{Cu}_2\text{Co}_2\text{SOD}$. histidine-44 is detached upon anion binding, **J. Am. Chem. Soc.**, 109, 2328-2334, 1987

157. Banci, L., Bertini, I., Gallori, E., Luchinat, C., Paoletti, F., Polsinelli, M., and Viezzoli, M. S., A spectroscopic investigation of cobalt(II) substituted alkaline phosphatase, **J. Inorg. Biochem.**, 30, 77-85, 1987

158. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., and Scozzafava, A., Characterization of the cobalt(II)-substituted superoxide dismutase-phosphate system, **Inorganic Chemistry**, 26, 153-156, 1987

159. Bertini, I., Mangani, S., Messori, L., Mobilio, S., and Orioli, P. L., Structural features of the metal binding sites in transferrins by EXAFS and other spectroscopic techniques, in: *Biophysics and synchrotron radiation*, Bianconi, A. and Congiu Castellano, A., 176,

160. Bertini, I., Luchinat, C., and Monnanni, R., The enzyme carbonic anhydrase, in: *Carbon dioxide as a source of carbon*, Aresta, M. and Forti, G., 139,

161. Bertini, I., Luchinat, C., and Messori, L., Nuclear relaxation in NMR of paramagnetic systems, in: *Metal ions in biological systems*, vol. 21. Applications of nuclear magnetic resonance to paramagnetic species, Sigel, H., 47,

162. Bertini, I., Luchinat, C., Monnanni, R., Roelens, S., and Moratal Mascarell, J. M., Interaction of CO_2 and copper(II) carbonic anhydrase, **J. Am. Chem. Soc.**, 109, 7855-7856, 1987

163. 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

164. 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

165. 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 Co^{2+} and Ni^{2+} substituted concanavalin A and the Lentil and Pea Lectins, **J. Biol. Chem.**, 262, 16984-16994, 1987

166. Mota De Freitas, D., Luchinat, C., Banci, L., Bertini, I., and Valentine, J. S., ^{31}P NMR study of the interaction of inorganic phosphate with bovine copper-zinc superoxide dismutase, **Inorganic Chemistry**, 26, 2788-2791, 1987

167. Banci, L., Bertini, I., Luchinat, C., and Hallowell, R. A., An investigation of superoxide dismutase Lys-143, Ile-143, and Glu-143 mutants: $\text{Cu}_2\text{Co}_2\text{SOD}$ derivatives, **J. Am. Chem. Soc.**, 110, 3629-3633, 1988

168. Banci, L., Bertini, I., Luchinat, C., Monnanni, R., and Scozzafava, A., Water ^1H

- nuclear magnetic relaxation dispersion (NMRD) of Cu_2Zn_2 SOD with some anions and ^1H NMR spectra of $\text{Cu}_2\text{Co}_2\text{SOD}$ in the presence of CN^- , **Inorganic Chemistry**, 27, 107-109, 1988
169. 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
170. Banci, L., Bertini, I., Luchinat, C., Viezzoli, M. S., and Wang, Y., Characterization of Cu_2Co_2 - and Co_2Co_2 -alkaline phosphatase complexes at acidic pH, **Inorganic Chemistry**, 27, 1442-1446, 1988
171. Bertini, I., Hirose, J., Kozlowski, H., Luchinat, C., Messori, L., and Scozzafava, A., Effect of nonsynergistic anions on copper transferrin, **Inorganic Chemistry**, 27, 1081-1086, 1988
172. Bertini, I., Messori, L., Pellacani, G. C., and Sola, M., Evidence of metal-synergistic anion bond in thallium(III) transferrin, **Inorganic Chemistry**, 27, 761-762, 1988
173. 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
174. 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
175. Bertini, I., Banci, L., and Luchinat, C., NMR of paramagnetic systems: magnetically coupled dimetallic systems. Cu_2Co_2 -superoxide dismutase as an example, in: Metal clusters in proteins, Que, L., Jr., 70,
176. Bertini, I., Hirose, J., Luchinat, C., Messori, L., Piccioli, M., and Scozzafava, A., Kinetic studies on metal removal from transferrins by pyrophosphate, **Inorganic Chemistry**, 27, 2405-2409, 1988
177. 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
178. 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, **Inorganic Chemistry**, 27, 951-953, 1988
179. Bertini, I., Monnanni, R., Pellacani, G. C., Sola, M., Vallee, B. L., and Auld, D. S., ^{13}C NMR studies of carboxylate inhibitor binding to cobalt(II) carboxypeptidase A, **J.Inorg.Biochem.**, 32, 13-20, 1988
180. Bertini, I., Banci, L., Luchinat, C., and Hallewell, R. A., The exploration of the active-site cavity of copper-zinc superoxide dismutase, in: Annals of the New York academy of sciences, Blanch, H. W. and Klibanov, A. M., 37,
181. 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
182. 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
183. 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, **Inorganic Chemistry**, 27, 728-733, 1988
184. 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, **Inorganic Chemistry**, 27, 4458-4463, 1988
185. 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
186. 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
187. 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, **European Journal of Biochemistry**, 184, 125-129, 1989
188. Banci, L., Bertini, I., Luchinat, C., Piccioli, M., Scozzafava, A., and Turano, P., ¹H NOE studies on dicopper(II) dicobalt(II) superoxide dismutase, **Inorganic Chemistry**, 28, 4650-4656, 1989
189. Banci, L., Bertini, I., Luchinat, C., Scozzafava, A., and Turano, P., Binding of fluoride to copper zinc superoxide dismutase, **Inorganic Chemistry**, 28, 2377-2381, 1989
190. Bertini, I., Luchinat, C., Viezzoli, M. S., and Wang, Y., Active-site modification of SOD by H₂O₂ studied through ¹H NMR of the cobalt(II)-derivative, **Arch.Biochem.Biophys.**, 269, 586-594, 1989
191. Bertini, I., Banci, L., and Luchinat, C., ¹H NMR of paramagnetic metalloproteins, in: Nuclear Magnetic Resonance, Part B, Oppenheimer, N. J. and James, T. L., 246,
192. Bertini, I., Luchinat, C., Messori, L., and Vasak, M., Proton NMR spectra of the Co₄S₁₁ cluster in metallothioneins: a theoretical model, **J.Am.Chem.Soc.**, 111, 7300-7303, 1989
193. 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
194. 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
195. 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
196. 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, **Inorganic Chemistry**, 28, 352-358, 1989
197. 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
198. 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, **Inorganic Chemistry**, 28, 1490-1496, 1989
199. 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
200. Banci, L., Bertini, I., Luchinat, C., and Moratal Mascarell, J. M., The mechanism of action of carbonic anhydrase, in: Enzymatic and model carboxylation and reduction reactions for carbon dioxide utilization, Aresta, M. and Schloss, J. V., 181,
201. 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
202. 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
203. Banci, L., Bencini, A., Bertini, I., Luchinat, C., and Piccioli, M., ¹H NOE and ligand field studies of copper-cobalt superoxide dismutase with anions, **Inorganic Chemistry**, 29, 4867-4873, 1990
204. 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 Cu₂Co₂ derivative, **J.Inorg.Biochem.**, 39, 149-159, 1990
205. Banci, L., Bertini, I., Luchinat, C., and Piccioli, M., Transient versus steady state NOE in paramagnetic molecules. Cu₂Co₂SOD as an example, **FEBS Lett.**, 272, 175-180, 1990
206. Banci, L., Bertini, I., and Luchinat, C., The ¹H NMR parameters of magnetically coupled dimers - The Fe₂S₂ proteins as an example, **Struct.Bonding**, 72, 113-135,

1990

207. 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, **Inorganic Chemistry**, 29, 1438-1440, 1990
208. 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, **Inorganic Chemistry**, 29, 2398-2403, 1990
209. 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
210. Bertini, I., Briganti, F., and Luchinat, C., Double exchange versus J-inequality in $\text{Fe}_3\text{S}_4^\circ$ clusters, **Inorganica Chimica Acta**, 175, 9-10, 1990
211. 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
212. Bertini, I., Donaire, A., Messori, L., and Moratal Mascarell, J. M., Interaction of phosphate and pyrophosphate with cobalt(II) carboxypeptidase, **Inorganic Chemistry**, 29, 202-205, 1990
213. 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
214. 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*, **Inorganic Chemistry**, 29, 1874-1880, 1990
215. 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
216. 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, **Inorganic Chemistry**, 29, 1460-1463, 1990
217. 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
218. 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
219. Bertini, I., Briganti, F., and Scozzafava, A., Proton NMR spectroscopy of Flavocytochrome c_{552} from *Chromatium vinosum*, **Inorganic Chemistry**, 29, 3623-3625, 1990
220. 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
221. 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 Research Communications**, 12-13, 239-251, 1991
222. 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*, **Inorganica Chimica Acta**, 180, 171-175, 1991
223. 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, **Inorganic Chemistry**, 30, 4510-4516, 1991
224. 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 *Rhodocyclus gelatinosus*. A model for oxidized HiPIPs, **Inorganic Chemistry**, 30, 4517-4524, 1991
225. 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

226. 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

227. Banci, L., Bertini, I., Briganti, F., Luchinat, C., and Scozzafava, A., Iron-sulfur proteins: an insight into their electronic structure through ^1H NMR spectroscopy, in: Chemistry and properties of biomolecular systems, Rizzarelli, E. and Theophanides, T., 73,

228. Banci, L., Bertini, I., Luchinat, C., and Piccioli, M., Frontiers in NMR of paramagnetic molecules: ^1H NOE and related experiments, in: NMR and biomolecular structure, Bertini, I., Molinari, H., and Niccolai, N., 31,

229. 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

230. 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, **European Journal of Biochemistry**, 196, 123-128, 1991

231. Bertini, I., Banci, L., Luchinat, C., and Sola, M., The interaction of inhibitors with carbonic anhydrase, in: Carbonic Anhydrase, Botre', F. and Storey, B. T., 86,

232. 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

233. Bertini, I., Capozzi, F., Luchinat, C., and Turano, P., Applications of COSY to paramagnetic heme-containing systems, **J.Magn.Reson.**, 95, 244-252, 1991

234. Bertini, I. and Viezzoli, M. S., Superoxide dismutase: a Cu,Zn enzyme, in: Lectures in bioinorganic chemistry, Nicolini, M. and Sindellari, L., 125,

235. Bertini, I., Lepori, A., Luchinat, C., and Turano, P., Role of Arg-143 in human $\text{Cu}_2\text{Zn}_2\text{SOD}$ studied through anion binding, **Inorganic Chemistry**, 30, 3363-3364, 1991

236. 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

237. 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, **European Journal of Biochemistry**, 197, 691-697, 1991

238. 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

239. 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

240. 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

241. 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

242. 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

243. 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

244. Banci, L., Bertini, I., Turano, P., and Vicens Oliver, M., NOE and two-dimensional correlated ^1H NMR spectroscopy of cytochrome c' from *Chromatium vinosum*, **European Journal of Biochemistry**, 204, 107-112, 1992

245. Bertini, I., Luchinat, C., Pierattelli, R., and Vila, A. J., The interaction of acetate and

- formate with cobalt carbonic anhydrase. An NMR study, **European Journal of Biochemistry**, 208, 607-615, 1992
246. 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, **Inorganic Chemistry**, 31, 3975-3979, 1992
247. Bertini, I., Messori, L., and Viezzoli, M. S., Coordination compounds and life processes, **Coord.Chem.Rev.**, 120, 163-192, 1992
248. 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
249. 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
250. Bertini, I. and Luchinat, C., NMR of paramagnetic substances in solution, in: Physical methods for chemists, Drago, R. S., 500,
251. 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, **Inorganic Chemistry**, 31, 4433-4435, 1992
252. 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*, **European Journal of Biochemistry**, 204, 831-839, 1992
253. Bertini, I., Luchinat, C., and Xia, Z., Solvent water ^1H NMRD study of oxovanadium(IV) aquaion, **J.Magn.Reson.**, 99, 235-246, 1992
254. Bertini, I., Luchinat, C., and Xia, Z., Electron relaxation of titanium(III) hexaaqua complex detected by solvent water ^1H -NMRD spectroscopy, **Inorganic Chemistry**, 31, 3152-3154, 1992
255. 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, **Inorganica Chimica Acta**, 198-200, 483-491, 1992
256. 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
257. Banci, L., Bertini, I., Ciurli, S., Ferretti, S., Luchinat, C., and Piccioli, M., The electronic structure of $(\text{Fe}_4\text{S}_4)^{3+}$ clusters in proteins. An investigation of the oxidized high-potential iron-sulfur protein II from *Ectothiorhodospira vacuolata*, **Biochemistry**, 32, 9387-9397, 1993
258. 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
259. 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
260. 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
261. 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
262. Banci, L., Bertini, I., Capozzi, F., Ciurli, S., Gori Savellini, G., and Luchinat, C., NMR and MD Investigation on the Structure-Function Relationship in HiPIP, in: The development of science for the improvement of human life. Proceedings of the II Kyoto-Siena Symposium.,
263. 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
264. 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
265. Banci, L., Bertini, I., Marconi, S., and Pierattelli, R., ^1H NMR study of reduced heme proteins: myoglobin and cytochrome P450, **European Journal of Biochemistry**, 215, 431-437, 1993
266. Banci, L., Bertini, I., and La Penna, G., Molecular dynamics study on carboxypeptidase A: the effect of protonation of Glu 270, **Inorganic Chemistry**, 32, 2207-2211, 1993
267. Banci, L., Bertini, I., Luchinat, C., Messori, L., and Turano, P., Frontiers in 2D NMR of paramagnetic metalloproteins, **Applied Magnetic Resonance**, 4, 461-476, 1993
268. Banci, L., Bertini, I., Luchinat, C., and Viezzoli, M. S., pH dependent properties of SOD studied through mutants on Lys 136, **Inorganic Chemistry**, 32, 1403-1406, 1993
269. Bencini, A., Bertini, I., and Bini, T., Angular overlap interpretation of the spectromagnetic properties of the nitrate derivative of cobalt(II) substituted carbonic anhydrase, **Inorganic Chemistry**, 32, 3312-3315, 1993
270. Bertini, I., Capozzi, F., Luchinat, C., and Piccioli, M., ^1H NMR investigation of oxidized and reduced HiPIP from *R. globiformis*, **European Journal of Biochemistry**, 212, 69-78, 1993
271. Bertini, I., Hiromi, K., Hirose, J., Sola, M., and Viezzoli, M. S., Electron transfer between copper,zinc superoxide dismutase and $\text{Fe}(\text{CN})_6^{4-}$, **Inorganic Chemistry**, 32, 1106-1110, 1993
272. 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., **Magnetic Resonance in Chemistry**, 31, S17-S22, 1993
273. Bertini, I., Gori, G., Luchinat, C., and Vila, A. J., 1D and 2D NMR characterization of oxidized and reduced cytochrome c' from *Rhodocyclus gelatinosus*, **Biochemistry**, 32, 776-783, 1993
274. Bertini, I., Ciurli, S., Dikiy, A., and Luchinat, C., The electronic structure of the $[\text{Fe}_4\text{Se}_4]^{3+}$ clusters in *Chromatium vinosum* HiPIP and *Ectothiorhodospira halophila* HiPIP II through NMR and EPR studies, **J.Am.Chem.Soc.**, 115, 12020-12028, 1993
275. 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
276. 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
277. Bertini, I., Briganti, F., Calzolari, L., Messori, L., and Scozzafava, A., Selective interaction of ferricyanide with cluster I of *Clostridium pasteurianum* $2[\text{Fe}_4\text{S}_4]$ ferredoxin, **FEBS Lett.**, 332, 268-272, 1993
278. Bertini, I., Capozzi, F., Luchinat, C., and Xia, Z., Nuclear and electron relaxation of $\text{Fe}(\text{OH}_2)_6^{3+}$, **J.Phys.Chem.**, 97, 1134-1137, 1993
279. Bertini, I., Briganti, F., Luchinat, C., and Xia, Z., Nuclear magnetic relaxation dispersion studies of hexaquo Mn(II) ions in water-glycerol mixtures, **J.Magn.Reson.**, 101, 198-201, 1993
280. 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
281. Bertini, I., Turano, P., and Vila, A. J., NMR of paramagnetic metalloproteins, **Chem.Rev.**, 93, 2833-2932, 1993
282. 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
283. Bertini, I., Luchinat, C., Messori, L., and Vasak, M., A two-dimensional NMR study of cobalt(II) $_7$ rabbit liver metallothionein, **European Journal of Biochemistry**, 211, 235-

240, 1993

284. 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*, **Applied Magnetic Resonance**, 4, 477-489, 1993

285. 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.Comm.**, 202, 1088-1095, 1994

286. 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, **European Journal of Biochemistry**, 225, 715-725, 1994

287. Banci, L., Bertini, I., and Luchinat, C., 2D NMR spectra of paramagnetic systems, in: *Methods in enzymology*, James, T. L. and Oppenheimer, N. J., 485,

288. Banci, L., Bertini, I., Cambria, M. T., Capozzi, F., and Dikiy, A., ¹H 1D and 2D NMR studies of the ferricytochrome c551 from *Rhodocyclus gelatinosus*, **European Journal of Biochemistry**, 219, 663-669, 1994

289. 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

290. Banci, L., Bertini, I., Pierattelli, R., and Vila, A. J., ¹H ¹³C HETCOR investigations on heme-containing systems, **Inorganic Chemistry**, 33, 4338-4343, 1994

291. Banci, L., Bertini, I., and La Penna, G., The enzymatic mechanism of carboxypeptidase: a molecular dynamics study, **Proteins: Structure, Function, and Genetics**, 18, 186-197, 1994

292. Benelli, B., Bertini, I., Capozzi, F., and Luchinat, C., ¹H NMR studies of the CoFe₃S₄ derivative of ferredoxin from *Clostridium acidi urici*. Dedicated to Prof. Luigi Sacconi, **Gazz.Chim.Ital.**, 124, 469-474, 1994

293. Bertini, I., Capozzi, F., Luchinat, C., Piccioli, M., and Vila, A. J., The Fe₄S₄ 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

294. 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, **Journal of Magnetic Resonance Series B**, B104, 95-98, 1994

295. Bertini, I., Felli, I. C., Kastrau, D. H. W., Luchinat, C., Piccioli, M., and Viezzoli, M. S., Sequence-specific assignment of the ¹H and ¹⁵N Nuclear Magnetic Resonance spectra of the reduced recombinant high potential iron sulfur protein (HiPIP) I from *Ectothiorhodospira halophila.*, **European Journal of Biochemistry**, 225, 703-714, 1994

296. 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 in Magnetic Resonance**, 6, 307-335, 1994

297. 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

298. Bertini, I. and Turano, P., The hyperfine coupling, in: *NMR of paramagnetic macromolecules*. NATO ASI Series., La Mar, G. N., 29,

299. Bertini, I., Luchinat, C., and Pierattelli, R., NMR and unpaired electrons in biomolecules, in: *NMR of biological macromolecules*. NATO ASI Series., Stassinopoulou, C. I., 199,

300. Bertini, I., Scozzafava, A., and Briganti, F., Specificity factors in metal ion-macromolecular ligand interactions vol.1, in: *Handbook on metal-ligand interactions of biological fluids*, Berthon, G.,

301. Bertini, I., Dikiy, A., Luchinat, C., Piccioli, M., and Tarchi, D., NOE-NOESY, a further tool in NMR of paramagnetic metalloproteins, **Journal of Magnetic Resonance Series B**, 103, 278-283, 1994

302. 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
303. 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
304. 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
305. Bertini, I., Luchinat, C., and Martini, G., Electron relaxation (data tabulation), in: Handbook of electron spin resonance, Poole, C. P., 79,
306. Bertini, I., Luchinat, C., and Martini, G., Electron relaxation (background and theory), in: Handbook of electron spin resonance, Poole, C. P., 51,
307. 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, **Journal of Magnetic Resonance Series B**, 104, 230-239, 1994
308. Bertini, I., Briganti, F., and Scozzafava, A., Zinc proteins interactions - zinc proteins, in: Handbook on metal-ligand interactions of biological fluids, Berthon, G.,
309. Bertini, I., Luchinat, C., and Piccioli, M., Copper zinc superoxide dismutase a paramagnetic protein that provides a unique frame for the NMR investigations, **Progress in Nuclear Magnetic Resonance Spectroscopy**, 26, 91-141, 1994
310. Bertini, I. and Luchinat, C., The reaction pathway of zinc enzymes and related biological catalysts, in: Bioinorganic chemistry, Bertini, I., Gray, H. B., Lippard, S. J., and Valentine, J. S., 37,
311. 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
312. 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, **European Journal of Biochemistry**, 232, 220-225, 1995
313. 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*, **Inorganica Chimica Acta**, 240, 251-256, 1995
314. Banci, L., Bertini, I., Chiu, C. Y., Mullenbach, G. T., and Viezzoli, M. S., Synthesis and characterization of a monomeric mutein of Cu/Zn superoxide dismutase with partially reconstituted enzymatic activity, **European Journal of Biochemistry**, 234, 855-860, 1995
315. 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
316. Banci, L., Bertini, I., Bren, K. L., Gray, H. B., Sompornpisut, P., and Turano, P., Three dimensional solution structure of the cyanide adduct of *Saccharomyces cerevisiae* Met80Ala-iso-1-cytochrome c. Identification of ligand-residue interactions in the distal heme cavity, **Biochemistry**, 34, 11385-11398, 1995
317. 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
318. Belinskii, M. I., Bertini, I., Galas, O., and Luchinat, C., The electronic structure of the Fe₄S₄³⁺ cluster in proteins: the importance of double exchange parameter. Dedicated to Prof. Hitoshi Ohtaki, **Zeitschrift für Naturforschung**, 50a, 75-80, 1995
319. 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

320. 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
321. Bertini, I., Donaire, A., Feinberg, B. A., Luchinat, C., Piccioli, M., and Yuan, H., Solution structure of the oxidized $2[\text{Fe}_4\text{S}_4]$ ferredoxin from *Clostridium pasteurianum*, **European Journal of Biochemistry**, 232, 192-205, 1995
322. 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
323. 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 & l'Industria**, 9, 639-648, 1995
324. 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
325. 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*, **Inorganic Chemistry**, 34, 2516-2523, 1995
326. 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
327. Bertini, I. and Viezzoli, M. S., NMR of paramagnetic molecules: a contribution to the understanding of enzymatic mechanisms. Nato ASI Series Kessissoglou, D. P., 93,
328. 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
329. 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
330. 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, **Inorganica Chimica Acta**, 235, 5-8, 1995
331. 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, **Journal of Magnetic Resonance Series A**, 113, 151-158, 1995
332. Bertini, I., Messori, L., and Viezzoli, M. S., Copper proteins, in: Handbook on metal-ligand interactions of biological fluids. New York, Berthon, G., 156,
333. Bren, K. L., Gray, H. B., Banci, L., Bertini, I., and Turano, P., pH dependent equilibria of Met80Ala-iso-1-cytochrome c probed by NMR spectroscopy; comparison with the WT protein, **Chemistry and Biology**, 2, 355-363, 1995
334. 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
335. Davy, S. L., Osborne, M. J., Breton, J., Moore, G. R., Thomson, A. J., Bertini, I., and Luchinat, C., Determination of the $(\text{Fe}_4\text{S}_4)\text{Cys}_4$ cluster geometry of *Desulfovibrio africanus* ferredoxin I by ^1H NMR spectroscopy, **FEBS Lett.**, 363, 199-204, 1995
336. 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
337. 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

338. Aono, S., Bertini, I., Cowan, J. A., Luchinat, C., Rosato, A., and Viezzoli, M. S., ^1H NMR studies of the Fe_7S_8 ferredoxin from *Bacillus schlegelii*: a further attempt to understand Fe_3S_4 clusters, **J.Biol.Inorg.Chem.**, 1, 523-528, 1996
339. Babini, E., Bertini, I., Borsari, M., Capozzi, F., Dikiy, A., Eltis, L. D., and Luchinat, C., A Serine \rightarrow Cysteine Ligand Mutation in the High Potential Iron-Sulfur Protein from *Chromatium vinosum* Provides Insight into the Electronic Structure of the $[\text{4Fe-4S}]$ Cluster, **J.Am.Chem.Soc.**, 118, 75-80, 1996
340. 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
341. 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
342. Banci, L., Bertini, I., Gori Savellini, G., and Luchinat, C., Individual Reduction Potentials of the Iron-Ions in Fe_2S_2 and high potential Fe_4S_4 ferredoxins, **Inorganic Chemistry**, 35, 4248-4253, 1996
343. Banci, L., Bertini, I., Quacquareni, G., Walter, O., Diaz, A., Hervás, M., and De la Rosa, M. A., The Solution structure of cytochrome c_6 the from green alga *monoraphidium braunii*, **J.Biol.Inorg.Chem.**, 1, 330-340, 1996
344. Banci, L., Bertini, I., Bruschi, M., Sompornpisut, P., and Turano, P., A NMR characterization and solution structure determination of the oxidized cytochrome c7 from *Desulfuromonas acetoxidans*, **Proc.Natl.Acad.Sci.USA**, 93, 14396-14400, 1996
345. Belinskii, M. I., Bertini, I., Galas, O., and Luchinat, C., An exchange coupling model for $\text{Fe}_4\text{S}_4^{3+}$ polymetallic center present in proteins and model compounds. Dedicated to Prof. H.B. Gray, **Inorganica Chimica Acta**, 243, 91-99, 1996
346. 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, **European Journal of Biochemistry**, 236, 92-99, 1996
347. 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
348. Bertini, I. and Luchinat, C., Electronic isomerism in oxidized Fe_4S_4 HiPIPs, in: Transition metal sulfur chemistry: biological and industrial significance, Stiefel, E. I. and Matsumoto, K., 57,
349. 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
350. Bertini, I., Luchinat, C., and Rosato, A., The solution structure of paramagnetic metalloproteins, **Progr.Biophys.Mol.Biol.**, 66, 43-80, 1996
351. 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 ba3*: an NMR investigation of the paramagnetic protein, **J.Am.Chem.Soc.**, 46, 11658-11659, 1996
352. Bertini, I., Donaire, A., Felli, I. C., Luchinat, C., and Rosato, A., From NOESY Cross-Peaks to Structural Constraints in a Paramagnetic Metalloprotein, **Magnetic Resonance in Chemistry**, 34, 948-950, 1996
353. 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, **Inorganic Chemistry**, 35, 6308-6315, 1996
354. Bertini, I., Briganti, F., Luchinat, C., and Scozzafava, A., Dioxygen activation in biodegradation reactions, **New J.Chem.**, 20, 187-193, 1996

355. 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
356. Bertini, I. and Luchinat, C., Experimental data and calculated parameters in FeS polymetallic centers in proteins, **J.Biol.Inorg.Chem.**, 1, 183-185, 1996
357. 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, **European Journal of Biochemistry**, 241, 440-452, 1996
358. 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
359. 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: Structure, Function, and Genetics**, 24, 158-164, 1996
360. Bertini, I. and Luchinat, C., Iron-sulfur proteins, in: Encyclopedia of Magnetic Resonance, Grant, D. M. and Harris, R. K., 2621,
361. 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
362. Bertini, I., A life with paramagnetic molecules, in: Encyclopedia of Magnetic Resonance, Grant, D. M. and Harris, R. K., 212,
363. 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, **Inorganic Chemistry**, 35, 1692-1700, 1996
364. 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
365. Banci, L., Bertini, I., Viezzoli, M. S., Argese, E., Orsega, E., Choi Ying Chiu, and Mullenbach, G. T., Tuning the activity of Cu₂Zn superoxide dismutase through site directed mutagenesis: a relatively active monomeric species, **J.Biol.Inorg.Chem.**, 2, 295-301, 1997
366. Banci, L., Bertini, I., Gori Savellini, G., Romagnoli, A., Turano, P., Cremonini, M. A., Luchinat, C., and Gray, H. B., The pseudocontact shifts as constraints for energy minimization and molecular dynamic calculations on solution structures of paramagnetic metalloproteins, **Proteins: Structure, Function, and Genetics**, 29, 68-76, 1997
367. 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
368. 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, **Magnetic Resonance in Chemistry**, 35, 845-853, 1997
369. 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
370. Banci, L., Bertini, I., Ferroni, F., and Rosato, A., Solution structure of reduced microsomal cytochrome *b₅*, **European Journal of Biochemistry**, 249, 270-279, 1997
371. 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
372. 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

373. 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
374. Bertini, I., Donaire, A., Luchinat, C., and Rosato, A., Paramagnetic relaxation as a tool for solution structure determination: *Clostridium pasterianum* ferredoxin as an example, **Proteins: Structure, Function, and Genetics**, 29, 348-358, 1997
375. 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
376. Bertini, I., Dikij, A., Luchinat, C., Macinai, R., Viezzoli, M. S., and Vincenzini, M., An NMR study of the 7Fe-8S ferredoxin from *Rhodospseudomonas palustris* and reinterpretation of data on similar systems, **Biochemistry**, 36, 3570-3579, 1997
377. Bertini, I., Gori Savellini, G., and Luchinat, C., Are unit charges always negligible?, **J.Biol.Inorg.Chem.**, 2, 114-118, 1997
378. Bertini, I., Donaire, A., Felli, I. C., Luchinat, C., and Rosato, A., ¹H and ¹³C NMR studies on an oxidized HiPIP, **Inorganic Chemistry**, 36, 4798-4803, 1997
379. Bertini, I. and Rosato, A., Solution structures of proteins containing paramagnetic metal ions, in: Molecular Modeling and Dynamics of Bioinorganic Systems, Banci, L. and Comba, P., 1,
380. 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
381. 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
382. 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, **European Journal of Biochemistry**, 258, 502-514, 1998
383. 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
384. 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
385. Arnesano, F., Banci, L., Bertini, I., and Felli, I. C., The solution structure of oxidized rat microsomal cytochrome b₅, **Biochemistry**, 37, 173-184, 1998
386. 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*, **European Journal of Biochemistry**, 256, 261-270, 1998
387. 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
388. Banci, L., Bertini, I., Turano, P., and Luchinat, C., The solution structure of redox proteins and beyond, in: Biological electron transfer chains: genetics and mode of operation, Canters, G. W. and Vijgenboom, E., 225,
389. 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
390. 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
391. 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, **European Journal of Inorganic Chemistry**, 1, 583-591, 1998
392. Banci, L., Bertini, I., De la Rosa, M. A., Koulougliotis, D., Navarro, J. A., and Walter,

- O., The solution structure of oxidized cytochrome c_6 from the green alga *Monoraphidium braunii*, **Biochemistry**, 37, 4831-4843, 1998
393. Banci, L., Bertini, I., Cavazza, C., Felli, I. C., and Koulougliotis, D., Probing the backbone dynamics of oxidized and reduced rat microsomal cytochrome b_5 via ^{15}N rotating frame NMR relaxation measurements: biological implications, **Biochemistry**, 37, 12320-12330, 1998
394. Banci, L., Bertini, I., Reddig, T., and Turano, P., Monitoring the conformational flexibility of cytochrome c at low ionic strength by ^1H NMR spectroscopy, **European Journal of Biochemistry**, 256, 271-278, 1998
395. 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
396. Banci, L., Bertini, I., Luchinat, C., Pierattelli, R., Shokhirev, N. V., and Walker, F. A., Analysis of the temperature dependence of the ^1H and ^{13}C 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
397. Banci, L., Bertini, I., Huber, J. G., Luchinat, C., and Rosato, A., Partial orientation of oxidized and reduced cytochrome b_5 at high magnetic fields: Magnetic susceptibility anisotropy contributions and consequences for protein solution structure determination, **J.Am.Chem.Soc.**, 120, 12903-12909, 1998
398. 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
399. 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
400. Bertini, I., Luchinat, C., Mincione, G., and Soriano, A., ^2H NMR Investigation of $[\text{Fe}_3\text{S}_4]^\circ$ cluster in 7Fe8S ferredoxin from *Bacillus schlegelii*, **Inorganic Chemistry**, 37, 969-972, 1998
401. Bertini, I., Mangani, S., and Viezzoli, M. S., Structure and properties of copper/zinc superoxide dismutases, in: *Advanced Inorganic Chemistry*, Sykes, A. G., 127,
402. Bertini, I., Luchinat, C., and Soriano, A., NMR of FeS proteins, in: *Spectroscopic methods in bioinorganic chemistry*, Solomon, E. I. and Hodgson, K. O., 302,
403. 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
404. Bertini, I., Luchinat, C., Parigi, G., Quacquarelli, G., Marzola, P., and Cavagna, F. M., Off-resonance experiments and contrast agents to improve magnetic resonance imaging, **Magnetic Resonance in Medicine**, 39, 124-131, 1998
405. Bertini, I., Luchinat, C., Piccioli, M., and Soriano, A., Folding properties of iron sulfur proteins. (Dedicated to Prof. O. Yamauchi), **Inorganica Chimica Acta**, 283, 12-16, 1998
406. Bertini, I., Luchinat, C., Macinai, R., Martinuzzi, S., Pierattelli, R., and Viezzoli, M. S., Isolation and characterization of a cytochrome c_2 from *Rhodopseudomonas palustris*. Dedicated to Prof. W.Beck, **Inorganica Chimica Acta**, 269, 125-134, 1998
407. 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
408. 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, **Inorganic Chemistry**, 37, 4814-4821, 1998
409. Im, S.-C., Liu, G., Luchinat, C., Sykes, A. G., and Bertini, I., The solution structure of parsley $[2\text{Fe}-2\text{S}]$ ferredoxin, **European Journal of Biochemistry**, 258, 465-477, 1998
410. Arnesano, F., Banci, L., Bertini, I., Felli, I. C., and Koulougliotis, D., Solution structure of the B form of oxidized rat microsomal cytochrome b_5 and backbone

- dynamics via ^{15}N rotating frame NMR relaxation measurements: Biological Implications, **European Journal of Biochemistry**, 260, 347-354, 1999
411. 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 *b*₅₆₂, **Biochemistry**, 38, 8657-8670, 1999
412. Assfalg, M., Banci, L., Bertini, I., Bruschi, M., Giudici-Ortoni, M. T., and Turano, P., A proton-NMR investigation of the fully reduced cytochrome *c*₇ from *Desulfuromonas acetoxidans*: comparison between the reduced and the oxidized forms, **European Journal of Biochemistry**, 266, 634-643, 1999
413. 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
414. 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
415. 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
416. 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
417. Banci, L., Bertini, I., Rosato, A., and Varani, G., Mitochondrial cytochromes *c*: a comparative analysis, **J.Biol.Inorg.Chem.**, 4, 824-837, 1999
418. 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
419. 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
420. Bertini, I., Luchinat, C., and Rosato, A., NMR spectra of iron-sulfur proteins, in: *Adv.Inorg.Chem.*, Sykes, A. G. and Cammack, R., 251,
421. Bertini, I., Rosato, A., and Turano, P., Solution structure of paramagnetic metalloproteins, **Pure and Applied Chemistry**, 71, 1717-1725, 1999
422. 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
423. 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
424. 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
425. Bertini, I., Clemente, A., Rombeck, I., Rosato, A., Turano, P., Lippert, B., and Quadrioglio, F., The three-dimensional solution structures of two DNA dodecamers through full relaxation matrix analysis, **Magnetic Resonance in Chemistry**, 37, 564-572, 1999
426. Bertini, I. and Luchinat, C., New Applications of Paramagnetic NMR in Chemical Biology, **Curr.Opin.Chem.Biol.**, 3, 145-151, 1999
427. 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
428. 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, 1999

429. 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 Dioxxygenase system, **Biochemistry**, 38, 11051-11061, 1999
430. 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
431. 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, **European Journal of Inorganic Chemistry**, 625-630, 2000
432. 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, unbonded 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
433. 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
434. Arnesano, F., Banci, L., Bertini, I., Karin van der Wetering, C., 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
435. 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
436. 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
437. 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., **European Journal of Biochemistry**, 267, 755-766, 2000
438. 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
439. 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
440. 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
441. 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
442. Bertini, I., Luchinat, C., and Rosato, A., The use of propionate α-proton contact shifts as structural constraints (Dedicated to Steve Lippard), **Inorganica Chimica Acta**, 297, 199-205, 2000
443. Bertini, I., Faraone-Mennella, J., Luchinat, C., and Rosato, A., The use of the electron-nucleus hyperfine interaction for solution structure determination, in: Metal-ligand interactions in chemistry, physics and biology, Russo, N. and Salahub, D. R., 1,
444. Bertini, I., Luchinat, C., and Turano, P., ¹⁵N chemical shift changes in cytochrome b₅: redox-dependent vs. guanidinium chloride-induced changes, **J.Biol.Inorg.Chem.**, 5, 761-764, 2000
445. 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

446. Bertini, I., Fernández, C. O., Karlsson, B. G., Leckner, J., Luchinat, C., Malmström, B. G., Nersissian, 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

447. Bertini, I., Fragai, M., Luchinat, C., and Parigi, G., ¹H NMRD profiles of diamagnetic proteins: a model-free analysis, **Magnetic Resonance in Chemistry**, 38, 543-550, 2000

448. 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: Structure, Function, and Genetics**, 41, 75-85, 2000

449. Bertini, I., Luchinat, C., and Parigi, G., The hyperfine shifts in low spin iron(III) hemes: a ligand field analysis, **European Journal of Inorganic Chemistry**, 2473-2480, 2000

450. 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, **European Journal of Biochemistry**, 267, 1008-1018, 2000

451. 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, **Inorganic Chemistry**, 39, 1755-1764, 2000

452. 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

453. 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

454. 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

455. 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

456. 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

457. Banci, L., Bertini, I., Felli, I. C., Hajjeva, 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

458. 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

459. Banci, L., Bertini, I., Branchini, B. R., Hajjeva, 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

460. Barker, P. B., Bertini, I., Del Conte, R., Ferguson, S. J., Hajjeva, P., Tomlinson, E. J., Turano, P., and Viezzoli, M. S., A further clue to understanding the mobility of mitochondrial yeast cytochrome c: a ¹⁵N T1ρ investigation of the oxidized and reduced species., **European Journal of Biochemistry**, 268, 4468-4476, 2001

461. 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

462. Bertini, I., Hajjeva, 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

463. Bertini, I., Fragai, M., Luchinat, C., and Parigi, G., Solvent ^1H NMRD Study of Hexaquochochromium(III): Inferences on Hydration and Electron Relaxation, **Inorganic Chemistry**, 40, 4030-4035, 2001
464. 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
465. 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
466. 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
467. 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
468. Bertini, I., Luchinat, C., and Piccioli, M., Paramagnetic Probes in Metalloproteins. Turning Limitations into Advantages, **Methods Enzymol.**, 339, 314-340, 2001
469. 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
470. 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
471. Dilg, A. W. E., Capozzi, F., Mentler, M., Iakovleva, O., Luchinat, C., Bertini, I., and Parak, F. G., Comparison and characterization of the $(\text{Fe}_4\text{S}_4)^{2+/3+}$ centre in the wild-type and C77S mutated HiPIPs from *Chromatium vinosum* monitored by Mössbauer, ^{57}Fe ENDOR and EPR spectroscopies, **J.Biol.Inorg.Chem.**, 6, 232-246, 2001
472. 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
473. 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
474. 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, **Inorganic Chemistry**, 40, 2111-2119, 2001
475. Muranyi, A. and Finn, B. E., Calcium and its enzymes, in: Handbook on Metalloproteins, Bertini, I., Sigel, A., and Sigel, H., 93,
476. Vila, A. J. and Fernández, C. O., Copper in electron-transfer proteins, in: Handbook on Metalloproteins, Bertini, I., Sigel, A., and Sigel, H., 813,
477. 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., **Inorganica Chimica Acta**, 331, 151-157, 2002
478. 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, **European Journal of Inorganic Chemistry**, 2121-2127, 2002
479. Antonkine, M. L., Liu, G., Bentrup, D., Bryant, D. A., Bertini, I., Luchinat, C., Stehlik, D., and Golbeck, J. H., Solution Structure of the unbound, photosystem I subunit PsuC, containing $[\text{4Fe-4S}]$ clusters F_A and F_B . A conformational change occurs upon binding to photosystem I, **J.Biol.Inorg.Chem.**, 7, 461-472, 2002
480. 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

481. Arnesano, F. and Bertini, I., Structural genomics on metalloproteins., **Gene Function and Disease**, 3, 1337-1347, 2002
482. 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
483. 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
484. 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
485. 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
486. 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
487. 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
488. 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
489. 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
490. 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).
491. 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 Science**, 11, 2479-2492, 2002
492. 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
493. 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
494. Bartalesi, I., Bertini, I., Hajieva, P., Rosato, A., and Vasos, P. R., Solution structure of a mono-heme ferrocycytochrome *c* from *Shewanella putrefaciens* and structural analysis of sequence-similar proteins: functional implications., **Biochemistry**, 41, 5112-5119, 2002
495. 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).
496. 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
497. Bertini, I., Luchinat, C., and Parigi, G., Magnetic susceptibility in paramagnetic NMR, **Progress in Nuclear Magnetic Resonance Spectroscopy**, 40, 249-273, 2002
498. 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
499. 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: Structure, Function, and Genetics**, 46, 110-127, 2002
500. 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
501. Bertini, I., Luchinat, C., and Parigi, G., Paramagnetic constraints: an aid for quick solution structure determination of paramagnetic metalloproteins, **Concepts in Magnetic Resonance**, 14, 259-286, 2002
502. Bertini, I., Longinetti, M., Luchinat, C., Parigi, G., and Sgheri, L., Efficiency of paramagnetism-based constraints to determine the spatial arrangement of α-helical secondary structure elements, **J.Biomol.NMR**, 22, 123-136, 2002
503. 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
504. 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).
505. Arnesano, F., Banci, L., Bertini, I., Felli, I. C., Luchinat, C., and Thompson, 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).
506. Arnesano, F., Banci, L., Bertini, I., Mangani, S., and Thompson, 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).
507. 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).
508. 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).
509. 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).
510. 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).
511. Banci, L., Bertini, I., Cramaro, F., Del Conte, R., and Viezzoli, M. S., Solution structure of apo Cu,Zn superoxide dismutase: the role of metal ions in protein folding., **Biochemistry**, 42, 9543-9553, 2003 (IF 4.064).
512. 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).
513. 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).
514. 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).
515. 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).
516. 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).
517. 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).
518. 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).
519. 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).
520. Bermel, W., Bertini, I., Felli, I. C., Kümmerle, 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
521. 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).
522. Bertini, I., Luchinat, C., and Sola, M., Zinc enzymes/models, **Encyclopaedia of Chemistry**, DOI: 10.1002/0471227617.EOC205, 2003
523. 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).
524. Bertini, I., Structural genomics., **Acc.Chem.Res.**, 36, 155-, 2003 (IF 15.901).
525. 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).
526. 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
527. Bertini, I., Capozzi, F., and Luchinat, C., Electronic isomerism in oxidized HiPIPs revisited, **ACS series**, 858, 272-286, 2003
528. Bertini, I., Luchinat, C., Turano, P., Battaini, G., and Casella, L., The magnetic properties of myoglobin as studied by NMR., **Chemistry - A European Journal**, 9, 2316-2322, 2003 (IF 4.238).
529. 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).
530. 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).
531. 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).
532. 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).
533. 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).
534. 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).

535. Andreini, C., Bertini, I., and Rosato, A., A hint to search for metalloproteins in gene banks, **Bioinformatics**, 20, 1373-1380, 2004 (IF 6.701).

536. 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).

537. Arnesano, F. and Bertini, I., Molecular basis of metal-ion selectivity and ultrasensitivity of metalloregulatory proteins, **Chem.Tracts**, 17, 2004

538. 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).

539. Arnesano, F., Banci, L., Bertini, I., and Ciofi-Baffoni, S., Perspectives in inorganic structural genomics: a trafficking route for copper, **European Journal of Inorganic Chemistry**, 2004, 1583-1593, 2004 (IF 2.482).

540. Babini, E., Bertini, I., Capozzi, F., Del Bianco, C., Holleder, 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).

541. 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).

542. 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).

543. 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).

544. 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).

545. Banci, L., Bertini, I., Cantini, F., Ciofi-Baffoni, S., Gonnelli, L., and Mangani, S., Solution structure of Cox11: a novel type of β -immunoglobulin-like fold involved in CuB site formation of cytochrome c oxidase, **J.Biol.Chem.**, 279, 34833-34839, 2004 (IF 6.482).

546. Banci, L., Bertini, I., Borrelly, G. P. M., Ciofi-Baffoni, S., Robinson, N. J., and Su, X. C., Solution structures of a cyanobacterial metallochaperone: insight into an atypical copper binding motif, **J.Biol.Chem.**, 279, 27502-27510, 2004 (IF 6.482).

547. 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).

548. 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).

549. 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).

550. Bertini, I., Faraone-Mennella, J., Gray, B. H., Luchinat, C., Parigi, G., and Winkler, J. R., NMR-validated structural model for oxidized *Rhodospseudomonas palustris* cytochrome c556, **J.Biol.Inorg.Chem.**, 9, 224-230, 2004 (IF 3.905).

551. 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).

552. 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).

553. Bertini, I. and Pierattelli, R., Copper(II) proteins are amenable for NMR investigation, **Pure and Applied Chemistry**, 76, 321-333, 2004 (IF 1.471).
554. Bertini, I., Felli, I. C., Kümmerle, R., Moskau, D., and Pierattelli, R., ^{13}C - ^{13}C NOESY: an attractive alternative to study large macromolecules, **J.Am.Chem.Soc.**, 126, 464-465, 2004 (IF 6.516).
555. 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).
556. 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).
557. Bertini, I. and Rosato, A., A genomic frontier in bioinorganic chemistry, **Chem.Lett.**, 33, 946-951, 2004 (IF 1.579).
558. 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).
559. 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).
560. 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).
561. 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., **Magnetic Resonance in Chemistry**, 41, 615-621, 2004 (IF 1.265).
562. Desvaux, H., Kümmerle, R., Kowalewski, J., Luchinat, C., and Bertini, I., Direct measurement of dynamic frequency shift of cross-correlation in ^{15}N enriched proteins, **Chem.Phys.Chem.**, 5, 959-965, 2004 (IF 2.070).
563. Andreini, C., Banci, L., Bertini, I., Elmi, S., and Rosato, A., A comparative analysis of the ADAM and ADAMTS families, **J.Proteome Res.**, 4, 881-888, 2005 (IF 6.917).
564. 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).
565. 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).
566. 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, **Angew.Chem.Int.Ed.**, 39, 6341-6344, 2005 (IF 9.161).
567. 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).
568. 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).
569. 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).
570. 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).
571. 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).
572. 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).
573. 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).
574. 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).
575. 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).
576. 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).
577. 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).
578. 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, 13-5-2005 (IF 9.161).
579. 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).
580. 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).
581. 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, **Journal Medicine Chemistry**, 48, 7544-7559, 2005 (IF 5.076).
582. Bertini, I., Luchinat, C., Parigi, G., and Pierattelli, R., NMR of paramagnetic metalloproteins, **ChemBioChem**, 6, 1536-1549, 2005 (IF 3.474).
583. 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, 2-4, 2005 (IF 9.161).
584. 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).
585. Bertini, I., Jiménez, B., Piccioli, M., and Poggi, L., Asymmetry in ¹³C-¹³C COSY spectra identifies geometry in paramagnetic proteins, **J.Am.Chem.Soc.**, 127, 12216-12217, 9-7-2005 (IF 6.903).
586. Bertini, I., Jiménez, B., and Piccioli, M., ¹³C direct detected experiments: optimisation to paramagnetic signals, **J.Magn.Reson.**, 174, 125-132, 1-5-2005 (IF 2.461).
587. Ab, E., Atkinson, A. R., Banci, L., Bertini, I., Ciofi-Baffoni, S., Brunner, K., Diercks, T., Doetsch, 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., Wohnert, J., Zweckstetter, M., and Kaptein, R., NMR in structural proteomics, **Acta Crystallogr D**

Biol Crystallogr, 62, 1161-, 2006 (IF 1.401).

588. 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).

589. Albeck, S., Alzari, P., Andreini, C., Banci, L., Berry, I. M., Bertini, I., Cambillau, C., Canard, B., Carter, L., Cohen, S.X., Diprose, J.M., Dym, O., Esnouf, R.M., Felder, C., Ferron, F., Guillemot, F., Hamer, R., Ben Jelloul, M., Laskowski, R.A., 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).

590. 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).

591. 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).

592. 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).

593. 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).

594. Balayssac, S., Bertini, I., Luchinat, C., Parigi, G., and Piccioli, M., ¹³C direct detected NMR increases the detectability of residual dipolar couplings, **J.Am.Chem.Soc.**, 128, 15042-15043, 2006 (IF 7.419).

595. 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).

596. 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).

597. 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

598. 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. Erratum in: Proc Natl Acad Sci U S A. 2006 Aug 1;103(31):11814, 2006 (IF 10.231).

599. 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).

600. 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).

601. 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).

602. 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).
603. Bermel, W., Bertini, I., Felli, I. C., Piccioli, M., and Pierattelli, R., ^{13}C -detected *protonless* NMR spectroscopy of proteins in solution, **Progress in Nuclear Magnetic Resonance Spectroscopy**, ⁴⁸, 25-45, 2006 (IF 6.462).
604. Bermel, W., Bertini, I., Felli, I. C., Kümmerle, 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).
605. Bertini, I., Grassi, E., Luchinat, C., Quattrone, A., and Saccenti, E., Monomorphism of human Cytochrome *c*, **Genomics**, 88, 669-672, 2006 (IF 3.181).
606. 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).
607. Bertini, I., Cavallaro, G., and Rosato, A., Cytochrome *c*: occurrence and functions, **Chem.Rev.**, 106, 90-115, 2006 (IF 20.869).
608. Bertini, I., Felli, I. C., Gonnelli, L., Pierattelli, R., Spyranti, Z., and Spyroulias, G. A., Mapping protein-protein interaction by ^{13}C -detected heteronuclear NMR spectroscopy, **J.Biomol.NMR**, 36, 111-122, 2006 (IF 2.18).
609. 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).
610. Pintacuda, G., Giraud, N., Pierattelli, R., Böckmann, A., Bertini, I., and Emsley, L., Solid-state NMR of a paramagnetic protein: assignment and study of the human dimeric oxidized Cu(II), Zn(II) superoxide dismutase, **Angew.Chem.Int.Ed.**, 46, 1079-1082, 2006 (IF 9.596).
611. Andreini, C., Banci, L., Bertini, I., Elmi, S., and Rosato, A., Non-heme iron through the three domains of life, **Proteins**, 2007 (IF 4.684) In Press
612. Balayssac, S., Bertini, I., Lelli, M., Luchinat, C., and Maletta, M., Paramagnetic ions provide precious structural restraints in solid-state NMR of proteins, **J.Am.Chem.Soc.**, 2007 (IF 7.419) In Press
613. 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 (IF10.231).
614. 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.**, 2007 (IF 6.901) In Press
615. Banci, L., Bertini, I., Cavallaro, G., and Rosato, A., The functions of Sco proteins from genome-based analysis, **J.Proteome Res.**, 2007 (IF 6.901) In Press
616. Bertini, I., Cavallaro, G., and Rosato, A., Evolution of mitochondrial-type cytochrome *c* and of the protein machinery for their assembly, **J.Inorg.Biochem.**, 2007 (IF 2.423) In Press
617. Bertini, I., Calderone, V., Fragai, M., Giachetti, A., Loconte, M., Luchinat, C., Maletta, M., Nativi, C., and Yeo, K. J., Understanding the Fine Tuning of Drug-receptor interactions: the Case of Matrix Metalloproteinases, **J.Am.Chem.Soc.**, 2007 (IF 7.419) In Press
618. Coyne, H. J., Ciofi-Baffoni, S., Banci, L., Bertini, I., Zhang, L., Graham, N. G., and Winge D.E., The characterization and the role of zinc binding in yeast cox4, **J.Biol.Chem.**, epub ahead of print, 2007 (IF 5.854).

BOOKS

1. Bertini, I. and Luchinat, C. NMR of paramagnetic molecules in biological systems, Menlo Park, CA: Benjamin/Cummings, 1986.
2. Banci, L., Bertini, I. and Luchinat, C. Nuclear and electron relaxation. The magnetic nucleus-unpaired electron coupling in solution, Weinheim: VCH, 1991.
3. Bertini, I. and Luchinat, C. NMR of paramagnetic substances, Amsterdam:

Coord.Chem.Rev. 150, Elsevier, 1996. Ed.1 pp. 1-300.

4. Bertini, I.; Luchinat, C.; Parigi, G.; Solution NMR of paramagnetic molecules. Applications to metalloproteins and models, Currents Methods in Inorganic Chemistry vol.2, Elsevier, 2001.

BOOKS AND SPECIAL VOLUMES EDITED

5. ESR and NMR of Paramagnetic Species in Biological Systems, Dordrecht: Reidel, 1980.
6. Koenig, S.H. and Brown III, R.D. ESR and NMR of Paramagnetic Species in Biological and Related System, edited by Bertini, I. and Drago, R.S. Dordrecht: Reidel, 1980, p. 89
7. Advances in Solution Chemistry, Plenum Press, 1981.
8. Coordination Chemistry Review, Amsterdam: Elsevier, 1982. pp. vol.43
9. Coordination Chemistry of Metalloenzymes, Dordrecht: Reidel, 1983.
10. Zinc Enzymes, Boston: Birkhauser, 1986.
11. NMR and Biomolecular Structure, Weinheim: VCH, 1990.
12. Coordination Chemistry Review, Amsterdam: Elsevier, 1992. pp. vol.120
13. Bertini, I. Magnetic Resonance in Chemistry, John Wiley, 1993.
14. Bioinorganic Chemistry, Mill Valley, CA: University Science Books, 1994.
15. Coordination Chemistry Reviews, Canada: Elsevier, 1999.
16. Handbook on Metalloproteins, edited by Bertini, I.; Sigel, A.; Sigel, H.; Marcel Dekker, Inc.; Basel, Switzerland, 2001.

BOOKS IN ITALIAN

17. Bertini, I. and Mani, F. Stechiometria, Milano: CEA, 1972.
18. Bertini, I. and Mani, F. Lezioni di chimica, Padova: CEA, 1976.
19. Enciclopedia della Chimica, ISEDI, 1977.
20. Bertini, I. and Mani, F. Chimica inorganica con nozioni di chimica organica, Padova: CEDAM, 1979.
21. Bertini, I. and Mani, F. Chimica inorganica con nozioni di chimica bioinorganica, Padova: CEDAM, 1988.
22. Bertini, I., Luchinat, C. and Rosato, A. Principi di chimica al calcolatore, Milano: Sorbona, 1995.
23. Bertini, I., Luchinat, C. and Mani, F. Chimica, CEA, 2004