

IVANO BERTINI
Curriculum Vitae (March 2009)

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Ivano Bertini was born in 1940 in Pisa, Italy, obtained the Italian degree of Doctor in Chemistry at the University of Florence in 1964 and then the Libera Docenza in 1969. He became full professor in General and Inorganic Chemistry in 1975 at the University of Florence where he is now. He received the Laurea Honoris Causa from the University of Stockholm in 1998, Ioannina in 2002 and Siena in 2003. Member of the Academia Europaea and of the Italian Accademia dei Lincei, he is or has been in the editorial staff or advisory board of about 20 among the most authoritative journals in chemistry, biochemistry and inorganic chemistry.

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

In 1999 he founded the present Center of Magnetic Resonance (CERM) of 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 life sciences. Flanking institutions and spin off laboratories have flourished around CERM in the fields of biotechnology and drug discovery thanks to his inspiring action.

Place and Date of birth: Pisa, December 6, 1940

Degree: Doctorate in Chemistry, 110/110 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
Eraldo Antonini Lifetime Achievement Award in Metalloproteins, Rome 2006
Basolo Medal, Evanston, IL, USA 2006
Cannizzaro Medal, Florence 2006
Fellowship of ISMAR, the International Society for Magnetic Resonance 2008

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
Special Lecturer Basolo, Northwestern University, Evanston, IL, USA 2006
Swift Lecture, CALTECH, Pasadena, CA, USA 2007

Society Memberships: Italian Chemical Society, American Chemical Society, Society of Biological Inorganic Chemistry.

Involvement in Scientific Journals (member of boards)

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 1999-2006
Accounts of Chemical Research, 1998-1999, Consulting Editor 1999-
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-
Open Inorganic Chemistry Journal, 2007-
Metallomics 2007-
FEBS 2008-

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 Advances in Inorganic Chemistry, 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. Fajta, 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;
- Vicepresident 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 of the no profit organization Fondazione Farmacogenomica Fiorgen 2003
- Co-founder of the University Spin off company ProtEra 2003
- Member of Working Group ESFRI on Research Infrastructure for Biology and Medical Science 2004-2007
- Chair of the Working Party on Chemistry in Life Sciences of European Chemical Societies EUCHEMS, 2004
- Founder 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 metalloproteins 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 popularise 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; Euechem 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; Greece-Italy-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; Central European Conference on "Chemistry Towards Biology", Portoroz, Slovenia 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, Okazaky, Japan 2003; Ohtaki Symposium, Kusatsu, Japan 2003; NMR in molecular Biology, Obernay, 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 on 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; VIth 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; 5th Hellenic Forum on Bioactive Peptides, Patras (Greece) 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 therapeutical effects, Montecatini, Italy, 2006; ICMRBS XXII Goettingen, Germany 2006, VIII Central European NMR symposium Debrecen, Hungary 2006; 3rd Asian Biological Inorganic Chemistry Conference, Nanjing, (P.R. China) 2006; ICBIC XIII, Wien, (Austria) 2007; Symposium Antonio Xavier, Oeiras, (Portugal) 2007, II European Conference on Chemistry for Life Sciences, Wroclaw (Poland) 2007; Symposium on Future Perspectives of Biomolecular NMR, Munich (Germany) 2008, 26th CCS 2008, Tianjin, (China) 2008, ACS meeting, Philadelphia (USA) 2008; IV Chemistry Towards Biology, Budapest, (Ungary) 2008; 2nd Annual RIMED Lecture, Rome (Italy) 2008; Magnetic Moments in Central Europe, Otocec (Slovenia) 2009

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 Münster, (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, University of Crete, Heraklion (CRETE) 2007, NMR EMBL Heidelberg (Germany) 2009; University of Basel, Basel, (Switzerland) 2009.

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; University of Verona, 2007; Mario Negri Institute, Milano 2008.

Organization of Congresses

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;
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;
1st Swiss-Italian Symposium, Bressanone, 1981;

First International Conference on Bioinorganic Chemistry, Florence, 1983 and the moving spirit behind the series;

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, 11th of the series with A. Gaslund, Stockholm University, Sweden, Vallombrosa 2007. All the Chianti Workshops were organized with the University of Pisa and Siena.

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 co-organizer 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;

Chairman of the Organizing Committee of the 3rd, 7th Eurasia Conference on Chemistry, Bangkok 1992 and 8th in Hanoi, Vietnam 2003

Chairman of the workshop on Bioinorganic and Biotechnological Aspects of Environmental Chemistry, Florence 1992;

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

Chairman of the 2nd Eurobic Conference, Florence 1994;

Chairman of the European Research Conference on "Chemistry of Metals in Biological Systems", San Miniato, 1995;

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

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

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

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

Round Table on "Worldwide network in NMR Structural Biology in the Post-Genomic Era", Florence, 1999;

Organizer of 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;

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

Chairperson of the XIX International Conference on Magnetic Resonance in Biological Systems, Florence, 2000.

Chair of the 10th International Conference on Bioinorganic Chemistry, Florence 2001.

Organizer of the 1st Central European Conference "Chemistry Towards Biology", Portoroz, Slovenia 2002

Organizer of the 6th European NMR Large Scale Facilities User Meeting, Montecatini, 2002.

Chairman of the International Conference on Genome-Based Drug Discovery, Florence 2004.
Chair of the First European Conference on Chemistry for Life Sciences, Rimini 2005.
Co-organizer of the 1st European Chemistry Congress, Budapest, Hungary 2006.
Co-organizer of the Advances and Management of NMR in Life Sciences, Florence 2007
(<http://www.cerm.unifi.it/EUNMR2007/>)
Co-organizer of the Perspectives of NMR in Drug Discovery, Florence 2007
(<http://www.cerm.unifi.it/NMRDD/>)

Member of the **international organizing committee** of the:
ICBIC 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 and Cairns 2003.

Second, third, fourth and fifth **Italian--Swiss Symposium**, Fribourg 1983, Ferrara 1986, Neuchâtel 1988, Parma 1990. Then this involved into the Eurobic series.

Eurobic First (Newcastle upon Tyne) 1992 and third (Wageningen) 1996.

Eurasia 1st to 6th Conference on Chemistry, Bangkok, 1988, Seoul 1990, Bangkok 1992, Kuala Lumpur, 1994, Guangzhou, China 1996; Brunei 2000, Karachi, Pakistan 2002.

Italian-Portuguese-Spanish meeting on Inorganic Chemistry, Gandia 1990, Albufeira 1992, Senigallia 1995.

Coorganizer of the **workshop on Peroxidases and Cyt P450**, Le Bischenberg, France 1992,

XVIII International Conference on Magnetic Resonance in Biological Systems, Tokyo, Japan 1998,

International Conference on **Structural Genomics** 2000, Yokohama, Japan 2000.

In addition he has been in the organizing committees of many other international and national conferences of Inorganic Chemistry, Biological Chemistry and related areas.

A 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 HCO_3^- 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 CO_2 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. Zeppezauer 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 ¹³C, ¹⁵N 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 Fe₄S₄ clusters, of one containing a Fe₃S₄ and one Fe₄S₄ cluster, of one containing a Fe₂S₂ 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 *c*3, *b*5 and *b*562. He then compared the mobility in the ms- μ s 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 500 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.