#### ANTONIO ROSATO

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#### Place and date of birth:

Florence, November 3<sup>rd</sup>, 1971

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# **Education:**

1995: Bachelor's degree in Chemistry (Degree: 110/110 cum laude and mention).

1995-1998: PhD in Chemical Sciences (University of Florence).

# **Career history:**

March 1999-June 1999: Bursary (Assegno di Ricerca) at the Department of Chemistry of the University of Florence

July 1999-October 2002: Assistant Professor at the Department of Chemistry of the University of Florence November 2002-Present: Associate Professor at the Department of Chemistry of the University of Florence

# Funded Projects (as Head of Research Unit or Workpackage Coordinator)

- WeNMR European Commission n. 261572
- INDIGO-Datacloud European Commission n. 653549
- MoBrain (EGI-ENGAGE) European Commission n. 654142
- PhenoMeNal European Commission n. 654241
- WeNMR Thematic Services (EOSC-HUB) European Commission n.777536
- EOSC-Life European Commission n. 824087

# **Boards**

Contributor to Faculty of 1000 (http://www.f1000biology.com/), 2010-2018

Scientific Data, Nature Publishing Group, Editorial Board member (<u>http://www.nature.com/scientificdata/</u>), 2017-present

International Journal of Molecular Sciences, MDPI, Editorial Board member (<u>https://www.mdpi.com/journal/ijms/sectioneditors/biochemistry</u>), 2018-present

Member of the Committee CES11-Characterization of structures and structure-function relationships of biological macromolecules of the French National Agency of Research, 2018-2020

# Honors:

VIII National Prize "FEDERCHIMICA - Per un Futuro Intelligente", 1996 Sapio NMR Junior Prize, 2001 Prize "Gastone de Santis" of the Division of Chemistry of Biological Systems of the Italian Chemical Society and Italfarmaco Inc., 2005

Prize "Raffaello Nasini" of the Division of Inorganic Chemistry of the Italian Chemical Society, 2009

# Meeting Organization:

"NMR for the Development of Science and Technology", Florence, 1996: member of the organizing committee

"XXXIII International Conference on Coordination Chemistry", Florence, 1998: member of the local organizing committee.

"3rd Meeting of the Users of the Large Scale Facilities for NMR in Life Sciences", Viareggio, 1999: member of the local organizing committee.

"XIX International Conference on Magnetic Resonance in Biological Systems", Florence 2000, coordinator of the national organizing committee.

"Workshop on Structural Genomics of the OECD Global Science Forum", Florence 2000, Scientific secretary

"New Challenges in the Life Sciences: Prioritizing European Research in Molecular Systems Biology", Florence 2007, member of the organizing committee.

"Strategies and Achievements of bio-NMR in Europe", San Diego, CA, 2008, member of the organizing committee

"Magnetic Resonance in the Life Sciences: What's New, Montecatini Terme, Italy, 2008, member of the organizing committee

"Structuring a Pan-European Bio-NMR Community", Firenze, Italy, 2009, organizer

"1st CASD-NMR Workshop", Firenze, Italy, 2010, organizer

"Joint EUROMAR and 17th ISMAR Conference, WWMR 2010, Florence, Italy, 2010, organizer

"From Molecular Structure to Systems Biology, S. Vito di Cadore, Italy, 2010, Member of the scientific committee

"WeNMR Workshop - Computational aspects of the joint use of SAXS and NMR", Florence, Italy, 2011, Organizer

"Advanced methods for the integration of other structural data with NMR data", Florence, Italy, 2013, Organizer

"National meeting of the Division of Chemistry of Biological Systems of the Italian Chemical Society", Bologna, Italy, 2013, Organizer

"National meeting of the Division of Chemistry of Biological Systems of the Italian Chemical Society", Syracuse, Italy, 2015, Organizer

Round Table "Bringing together the bio-medical scientific communities: the role of research infrastructures", Brno, Czech Republic, 2017, Organizer

INSTRUCT practical course on Advanced methods for the integration of diverse structural data (3rd edition), Florence, Italy, 2018, Organizer

# **Oral Presentations**

"7th Chianti Workshop on Magnetic Resonance", San Miniato 1997: Relaxation based constraints for solution structure determination of paramagnetic metalloproteins

"8th Chianti Workshop on Magnetic Resonance", San Miniato 1999: Partial orientation of cytochrome b5 at high fields: dissecting magnetic susceptibility anisotropy contributions

"11th ICBIC", Cairns, Australia 2003: Biological Inorganic Chemistry and Structural Genomics: can there be love?

"XXXIII National Congress on Magnetic Resonance", Bressanone 2003: A method to search for metalloproteins in gene banks

"<u>SPINE</u> workshop on NMR software tools", Regensburg, Germany, 2004: Structural constraints from paramagnetic effects

"CCPN/TEMBLOR Workshop on Data model driven approaches to software development", Hinxton, United Kingdom, 2004: Metalloprotein NMR structures and data storage

"VIth European Symposium of the Protein Society", Barcelona, Spain, 2005: Structure, function, dynamics and bioinformatics of metalloproteins

"III Congresso Nazionale della Divisione di Chimica dei Sistemi Biologici", Rimini, Italy, 2005: NMR and

bioinformatic studies of metalloproteins

"First European Conference on Chemistry for Life Sciences", Rimini, Italy, 2005: Identification of metalloproteins in the genome and their functional annotation

"Trends in Transient Interactions between Biological Macromolecules, Seville, Spain 2007: NMR studies of metal-mediated protein-protein interactions

"2nd European Conference on Chemistry for Life Sciences", Wroclaw, Poland 2007: Intracellular copper transport: a structural view

Round Table of the "EU-NMR Annual User Meeting", Frankfurt, Germany 2008: The eNMR project "2<sup>nd</sup> Biomed GRID School", Varenna, Italy 2008: The eNMR project

"Retreat of the North-East Structural Genomics, Consortium", Princeton, NJ, 2009: Recognizing Zn Binding Proteins in the Proteomes of Life

"2009 NIGMS Workshop – Enabling Technologies for Structural Biology", Bethesda, MD, 2009: The eNMR Platform For Structural Biology

"XXIII Congresso Nazionale della Società Chimica Italiana", Sorrento, Italy, 2009: Nasini Prize 2009, The roles of metal ions in cells: bioinformatic and experimental studies

"TOPIM 2010", Bardonecchia, Italy, 2010: Mechanistic systems biology of metal ions in cells

"The Biobank as an Instrument for Economic Development", Florence, Italy, 2010: GRID for Biobanks "Italian National NMR School", Torino, Italy, 2010: e-NMR and Automation

"18<sup>th</sup> EuroQSAR – EAST-NMR Satellite Meeting", Rhodes, Greece, 2010: The eNMR Platform for Structural Biology

"National School of Bioinorganic Chemistry", Siena, Italy, 2011: Metalloproteomics

"HealthGrid 2011", Bristol, United Kingdom, 2011: The WeNMR Platform for Structural Biology

"5th International Conference on Metals and Genetics", Kobe, Japan, 2011: Sequence- and structure-based analyses of metalloproteomes

"CECAM Workshop on Integrated Software for Integrative Structural Biology". Abingdon, United Kingdom, 2012: Exploring the conformational space of flexible multi-domain proteins by a combination of NMR and SAXS

"Seventh International Conference on Porphyrins and Phtalocyanines", Jeju island, Republic of Korea, 2012: Bioinformatics applied to heme-binding proteins: approaches and conclusions

"International Symposium on Grid and Clouds", Taipei, Taiwan, 2013: Automated NMR assignment and structure calculation

"18<sup>th</sup> ISMAR Meeting", Rio de Janeiro, Brazil, 2013: Conformational space of complexes from SAXS data – MAXOCC

"EGI Technical Forum", Madrid, Spain, 2013: Structural biology applications within WeNMR

"Modern Trends in Inorganic Chemistry XV", Roorkee, India, 2013: Structural bioinformatics of metalloproteins

"RDA Third Plenary Meeting", Dublin, Ireland, 2014: Open issues for structural biology data and metadata Invited seminar: Institut Pasteur, Paris, France, 2014: Bioinformatics and NMR studies of metalloproteins

"XXV National Congress of the Italian Chemical Society", Arcavacata di Rende, Italy, 2014: Structural bioinformatics of metalloproteins

"GLiB 2014 - Quarta Giornata Ligure di Bioinformatica", Genova, Italy, 2014: Structural bioinformatics of metalloproteins

"Research Infrastructures meet Research Data Alliance" Workshop, Amsterdam, The Netherlands, 2015: A distributed infrastructure for integrated structural biology

"EGI Conference 2016 - Opening science in Europe and in the World", Amsterdam, The Netherlands, 2016: The MoBrain Competence Center for Translational Research from Molecule to Brain

"Advanced methods for the integration of diverse structural data with NMR data  $-2^{nd}$  Edition" Training course, Amsterdam, The Netherlands, 2016: Molecular dynamics for NMR-based protein structure refinement

Invited seminar: Wageningen University, The Netherlands, 2016: The importance of metal sites for bioinformatics of metalloproteins

"CORBEL Annual General Meeting 2016", Graz, Austria, 2016: PhenoMeNal - Large Scale Computing for Medical Metabolomics

"FAIR Data Management: best practices and open issues", Florence, Italy, 2016: INSTRUCT, a distributed infrastructure for integrated structural biology

"International Symposium on Grids and Clouds", Taipei, Taiwan, 2017: Molecular dynamics of proteins in the cloud

"Data Management Services in the Cloud", Barcelona, Spagna, 2017: Molecular dynamics of proteins in the cloud

Invited seminar: Vrije Universiteit Bruxelles, Belgium, 2017: Bioinformatics of metalloproteins

"14th Annual Meeting of the Bioinformatics Italian Society", Cagliari, Italy, 2017: Tools and databases for bioinformatics of metalloproteins

"CloudMet 2017", Pula, Italy, 2017: Metabolic profiles for diagnostics/prognostics

"EOSC Stakeholder Forum, Brussels", Belgium, November 28-29, 2017. INSTRUCT-ERIC: requirements and possible contributions to the EOSC

"Digital Infrastructures For Research", Brussels, Belgium, Nov 30- Dec 1, 2017: Requirements for the use of structural biology (SB) data from the perspective of users and research infrastructures from neighboring fields

EBI Webinar, 17 Jul 2018: Metabolomics and Systems Biology

"46th National Conference on Inorganic Chemistry", Bologna, Italy, 10-13 Sep 2018: Bioinformatics and Molecular Dynamics of Metalloproteins

"Digital Infrastructures For Research 2018", Lisbona, Portogallo, 2018: WeNMR activities in the EOSC-Hub

"3<sup>rd</sup> CORBEL Annual General Meeting 2018", Paris, France, 2018: West-Life, a Virtual Research Environment for Structural Biology

"Past, present and future of inorganic chemistry in Italy: a path defined by the winners of the Nasini prize", Rome, Italy, 2019: Bioinformatics of Metalloproteins

"Scuola Nazionale di chimica bioinorganica per dottorandi 2019", Rome, Italy, 2019: How to apply bioinformatics to metalloproteins

"19th International Conference on Biological Inorganic Chemistry", Interlaken, Switzerland, 2019: Bioinformatics of Metalloproteins

"6th meeting of International Society for Zinc Biology (ISZB-2019)", Kyoto, Japan, 2019: Structural Bioinformatics of Zinc-binding Proteins

"Computational methods and NMR spectroscopy: a powerful synergy for chemistry, materials science and biology", Pisa, Italy, 2019: Evolutionary constraints in NMR-based protein structure determination

"CCP4 Study Weekend 2020", Nottingham, United Kingdom, 2020: The MetalPDB database

# Teaching duties (only at the Faculty of Sciences of the University of Florence):

2001/02-2003/04: Structural Chemistry (Degree in Chemistry).

2001/02-2006/07: General and Inorganic Chemistry (Degree in Chemistry and Degree in Applied Chemistry).

2004/2005-2006/07: Laboratory of Instrumental Technologies (Degree in Industrial and Environmental Biotechnology)

2005/2006-2006/07: Laboratory of biotechnology (Degree in Industrial and Environmental Biotechnology)

2005/2006-2006/07: Design and synthesis of biomolecules (Degree in Industrial and Environmental Biotechnology)

2002/03-2008/2009: Structure and reactivity of Biotechnological Macromolecules (Degree in Biotechnology).

2004/2005-2008/2009: Models of biological systems (Degree in Biotechnology).

2007/2008-2008/2009: Geobiochemical Cycles (Degree in Chemistry of Biological Molecules)

2009/2010-2011/2012: General and Inorganic Chemistry (Degrees in Biological Sciences, in Biotechnology and in Earth Sciences)

2009/2010–2010/2011: Bioinformatics and Computational Chemistry of Metalloproteins (2<sup>nd</sup> level Degree in Chemistry)

2004/2005-Present: Chemistry of Biodegradation Processes (2<sup>nd</sup> level Degree in Chemistry)

2012/2013-Present: Biomolecular structure (Degree in Biotechnology)

2018/2019-Present: Laboratory of Bioinformatics (2<sup>nd</sup> level Degree in Chemistry)

Dr. Rosato has held cycles of seminars for PhD students in Chemical Sciences and in Structural Biology. He is a member of the Board of Teachers of the PhD course in Structural Biology at the University of Florence.

He has chaired the self-evaluation team of the  $1^{st}$  and  $2^{nd}$  level Degrees in Chemistry from 2009 to 2017. He is a member of the Quality Assurance team of the whole University of Florence since 2020.

Books:Bertini, I., C. Luchinat, A. Rosato, Principi di Chimica al Calcolatore, Ed. Sorbona, Milan 1995.

Ph.D. Thesis supervised: Leonardo Decaria; Shailesh Sharma; Lucio Ferella; Davide Sala.

#### **Research activity**

The research activity of Antonio Rosato is focused on the investigation of metalloproteins, i.e. the proteins that need metals to perform their biological function. The main spectroscopic tool employed is nuclear magnetic resonance (NMR) in solution. Several publications of Dr. Rosato have addressed the development and application of advanced computational methods both for the experimental determination of metalloprotein structures, including paramagnetic NMR restraints, and for their bioinformatics analysis, through combinations of sequence/domain alignment and 3D structural modeling. At the beginning of his scientific career, Dr. Rosato investigated the effect of paramagnetic metal ions on

NMR spectra and how these effects can be exploited to obtain structural information on paramagnetic metalloproteins. This activity involved the development of new approaches to study chemical-physical effects on nuclear relaxation involving in particular nuclear spin-electron spin interactions. New software tools to quantify these effects and introduce them into structure calculation protocols were developed.

Dr. Rosato has been the scientific manager of an international collaboration funded by the European Commission (e-NMR, <u>www.enmr.eu</u>) that aimed at making software tools for the determination of the solution structure of proteins from NMR data available via the internet. The e-NMR activities have been continued in a number of different projects funded by the EC (e.g. WeNMR, <u>www.wenmr.eu</u>; West-Life, www.west-life.eu/), covering different aspects of the field of Structural Biology; Dr. Rosato was the P.I. of the University of Florence unit in the majority of these projects. In this context, Dr. Rosato launched and coordinated the international initiative "Critical Assessment of Automated Structure Determinarion by NMR (CASD-NMR)", which involved over a dozen teams of developers of software for biological NMR worldwide from 2009 to 2015. More recently, he was involved in the "Comparative Assessment of Structure Prediction (CASP)" initiative, as an assessor.

Another focus of the research activity of Dr. Rosato is the cellular mechanisms controlling the intracellular concentration and distribution of metal ions, in particular copper. These studies involved the investigation of protein-protein interactions, and the structural characterization of protein-protein adducts. Dr. Rosato contributed to the discovery of interactions that are driven by metal ions, a phenomenon that can be important in tuning various cellular processes (*metal-mediated protein-protein interactions*).

Finally, Dr. Rosato is involved in the application of bioinformatics methods to investigate the functional and structural response of metalloproteins to evolution and to changing environmental conditions. These studies exploit the comparative analysis of protein sequence and structures, starting from complete genome sequences, to obtain information on the biochemistry of the systems under study, their capability to bind different metal ions or to select among metal ions, and on the relevant reaction mechanisms. In this frame, new algorithms were developed to predict the metalloprotein content in proteomes. New software tools as well as on-line resources such as databases have been developed. An important achievement in this context was the implementation of the MetalPDB database (http://metalweb.cerm.unifi.it/).

On the whole, Dr. Rosato's studies contribute to the description of the role of essential metal ions in living systems and the characterization of the chemical and structural bases of that role. A second major goal is the development and provision of innovative computational methods for structural biology.

The h-index of Antonio Rosato is 42 (Web of Science) / 46 (Google Scholar).

#### List of Publications (including book chapters)

**1**. Aono, S., I. Bertini, J.A. Cowan, C. Luchinat, A. Rosato, M.S. Viezzoli. 1H NMR studies of the Fe7S8 ferredoxin from Bacillus schlegelii: a further attempt to understand Fe3S4 clusters. J. Biol. Inorg. Chem. 1: 523-528, 1996.

**2**. Banci, L., A. Rosato, P. Turano. Can the axial ligand strength be monitored through spectroscopic measurements? J. Biol. Inorg. Chem. 1: 364-367, 1996.

**3**. Bertini, I., M.M.J. Couture, A. Donaire, L.D. Eltis, I.C. Felli, C. Luchinat, M. Piccioli, A. Rosato. The Solution Structure Refinement of the Paramagnetic Reduced HiPIP I from Ectothiorhodospira halophila by Using Stable Isotope Labeling and Nuclear Relaxation. Eur.J.Biochem. 241: 440-452, 1996. [IF 3.275]

**4**. Bertini, I., I.C. Felli, C. Luchinat, A. Rosato. A Complete Relaxation Matrix Refinement of the Solution Structure of a Paramagnetic Metalloprotein: Reduced HiPIP I from E. halophila. Proteins Struct.Funct.Genet. 24: 158-164, 1996. [IF 4.374]

**5**. Bertini, I., C. Luchinat, A. Rosato. Evaluation of paramagnetic relaxation rates in a J-coupled two-spin system. Chem.Phys.Lett. 250: 495-504, 1996. [IF 2.589]

**6**. Bertini, I., A. Donaire, I.C. Felli, C. Luchinat, A. Rosato. From NOESY Cross-Peaks to Structural Constraints in a Paramagnetic Metalloprotein. Magn.Reson.Chem. 34: 948-950, 1996. [IF 1.009]

7. Bertini, I., C. Luchinat, A. Rosato. The solution structure of paramagnetic metalloproteins. Progr.Biophys.Mol.Biol. 66: 43-80, 1996. [IF 3.306]

**8**. Bertini, I., C. Luchinat, A. Rosato. Simulation of NMR spectra. In: NMR of Paramagnetic Substances, by I. Bertini and C. Luchinat. Coord. Chem. Rev. 150: 278-290, 1996.

**9**. Banci, L., I. Bertini, H.B. Gray, C. Luchinat, T. Reddig, A. Rosato, P. Turano. Solution structure of oxidized horse heart cytochrome c. Biochemistry 36: 9867-9877, 1997. [IF 4.572]

**10**. Banci, L., I. Bertini, F. Ferroni, A. Rosato. Solution structure of reduced microsomal cytochrome b5. Eur.J.Biochem. 249: 270-279, 1997. [IF 3.136]

**11**. Bertini, I., A. Donaire, C. Luchinat, A. Rosato. Paramagnetic relaxation as a tool for solution structure determination: Clostridium pasterianum ferredoxin as an example. Proteins Struct.Funct.Genet. 29: 348-358, 1997. [IF 4.161]

12. Bertini, I., A. Donaire, I.C. Felli, C. Luchinat, A. Rosato. 1H and 13C NMR studies on an oxidized HiPIP. Inorg.Chem. 36: 4798-4803, 1997. [IF 2.736]

**13**. Bertini, I. and Rosato, A. Solution structures of proteins containing paramagnetic metal ions. In: Molecular Modeling and Dynamics of Bioinorganic Systems, edited by Banci, L. and Comba, P. Dordrecht: Kluwer Academic Publishers, 1997, p. 1-19.

**14**. Aono, S., D. Bentrop, I. Bertini, A. Donaire, C. Luchinat, Y. Niikura, A. Rosato. Solution structure of the oxidized Fe7S8 ferredoxin from the thermophilic bacterium Bacillus schlegelii by 1H NMR spectroscopy. Biochemistry 37: 9812-9826, 1998. [IF 4.628]

**15**. Bertini, I., D.M. Kurtz, Jr., M.K. Eidsness, G. Liu, C. Luchinat, A. Rosato, R.A. Scott. Solution structure of reduced Clostridium pasteurianum rubredoxin. J. Biol. Inorg. Chem. 3: 401-410, 1998. [IF 4.412]

**16**. Banci, L., Bertini, I., Huber, J.G., Luchinat, C. Rosato, A. Partial orientation of oxidized and reduced cytochrome b5 at high magnetic fields: Magnetic susceptibility anisotropy contributions and consequences for protein solution structure determination, J. Am. Chem. Soc. 120: 12903-12909, 1998. [IF 5.725]

**17**. Arnesano, F., Banci, L., Bertini, I., Faraone-Mennella, J., Rosato, A., Barker, P.D., & Fersht, A.R. The Solution structure of oxidized Escherichia coli cytochrome b562, Biochemistry 38: 8657-8670, 1999. [IF 4.493]

**18**. Banci, L., Bertini, I., Rosato, A., & Varani, G. Mitochondrial cytochromes c: a comparative analysis, J. Biol. Inorg. Chem. 4, 824-837, 1999. [IF 4.464]

**19**. Bentrop, D., Bertini, I., Iacoviello, R., Luchinat, C., Niikura, Y., Piccioli, M., Presenti, C., & 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. [IF 4.493]

**20**. Bertini, I., Clemente, A., Rombeck, I., Rosato, A., Turano, P., Lippert, B., & Quadrifoglio, F. The three-dimensional solution structures of two DNA dodecamers through full relaxation matrix analysis, Magn.Reson.Chem. 37: 564-572, 1999. [IF 1.168]

**21**. Bertini, I., C. Luchinat, and A. Rosato NMR spectra of iron-sulfur proteins. In: Adv.Inorg.Chem. A.G. Sykes and R. Cammack, eds. Academic Press, San Diego, pp. 251-282, 1999.

**22**. Bertini, I., Rosato, A. & Turano, P. Solution structure of paramagnetic metalloproteins, Pure Appl.Chem. , 71: 1717-1725, 1999. [IF 1.141]

**23**. Banci, L., Bertini, I., Rosato, A., & Scacchieri, S. Solution structure of oxidized microsomal rabbit cytochrome b5. Factors determining the heterogeneous binding of the heme., Eur J Biochem 267: 755-766, 2000. [IF 2.852]

**24**. Bertini, I., J. Faraone-Mennella, C. Luchinat, and A. Rosato The use of the electron-nucleus hyperfine interaction for solution structure determination. In: Metal-ligand interactions in chemistry, physics and biology. N. Russo and D.R. Salahub, eds. Kluwer academic, Dordrecht, pp. 1-17, 2000.

**25**. Bertini, I., Luchinat, C., & Rosato, A. The use of propionate a-proton contact shifts as structural constraints (Dedicated to Steve Lippard), Inorg.Chim.Acta 297: 199-205, 2000. [IF 1.200]

**26**. Banci, L., Bertini,I., Cramaro F., Del Conte, R., & Rosato, A. 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, 2000. [IF 4.221]

**27**. Bertini, I., Janik, M.B.L., Liu, G., Luchinat, C., & 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. [IF 2.332]

**28**. Bertini, I., Janik, M.B.L., Lee, Y.-M., Luchinat, C., & Rosato, A. Magnetic Susceptibility Tensor Anisotropies for a Lanthanide Ion Series in a Fixed Protein Matrix, J. Am. Chem. Soc. 123: 4181-4188, 2001. [IF 6.079]

**29**. Banci, L., I. Bertini, S. Ciurli, A. Dikiy, J. Dittmer, A. Rosato, G. Sciara, A. Thompsett. NMR solution structure, backbone mobility and homology modeling of c-type cytochromes from gram-positive bacteria. ChemBioChem 3: 299-310, 2002. [IF 3.233]

**30**. Bartalesi, I., I. Bertini, P. Hajieva, A. Rosato, P. Vasos. Solution structure of a mono-heme ferrocytochrome c from Shewanella putrefaciens and structural analysis of sequence-similar proteins: functional implications. Biochemistry 41: 5120-5130, 2002. [IF 4.064]

**31**. Bertini, I., C. Luchinat, A. Provenzani, A. Rosato, P. Vasos. Browsing gene banks for Fe2S2 ferredoxins and structural modeling of 87 plant-type sequences: an analysis of fold and function. Proteins Struct.Funct.Genet. 46: 110-127, 2002. [IF 4.096]

**32**. Barbieri, R., I. Bertini, G. Cavallaro, Y.M. Lee, C. Luchinat, A. Rosato. Paramagnetically induced residual dipolar couplings for solution structure determination of lanthanide-binding proteins. J Am Chem Soc 124: 5581-5587, 2002. [IF 6.201]

**33**. Arnesano, F., L. Banci, P.D. Barker, I. Bertini, A. Rosato, X.C. Su, M.S. Viezzoli. Solution structure and characterization of the heme chaperone CcmE. Biochemistry 41: 13587-13594, 2002. [IF 4.096]

**34**. Bartalesi, I., I. Bertini, K. Ghosh, A. Rosato, P. Turano. The unfolding of oxidized c-type cytochromes: the instructive case of B. pasteurii. J Mol Biol 321: 693-701, 2002. [IF 5.359]

**35**. Banci L, Rosato A. Structural genomics of proteins involved in copper homeostasis. Acc.Chem.Res. 36:215-221, 2003 [IF 15.000]

**36**. Bartalesi I, Bertini I, 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]

**37**. Bertini I, Rosato A. Bioinorganic chemistry in the post-genomic era. Proc.Natl.Acad.Sci.USA 100:3601-3604, 2003 [IF 10.700]

**38**. Bertini I, Ghosh K, Rosato A, Vasos, PR. 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]

**39**. Banci L, Bertini I, Felli IC, Krippahl L, Kubicek K, Moura JJG, Rosato A. A further investigation of the cytochrome b5 - cytochrome c complex. J. Biol. Inorg. Chem. 8:777-786, 2003 [IF 3.911]

**40**. Bartalesi I, Rosato A, Zhang W. Hydrogen exchange in a bacterial cytochrome c: a fingerprint of the cytochrome c fold. Biochemistry, 42:10923-10930, 2003 [IF 4.064]

**41**. Andreini C, Banci L, Bertini I, Luchinat C, Rosato A. Bioinformatic Comparison of Structures and Homology-Models of Matrix Metalloproteinases J.Proteome.Res., 3:21-31, 2004 [IF 5.611]

**42**. Banci L, Bertini I, Del Conte R, D'Onofrio M, 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]

**43**. Andreini C, Bertini I, Rosato A. A hint to search for metalloproteins in gene banks. Bioinformatics, 20:1373-1380, 2004 [IF 6.701]

**44**. Bartalesi I, Bertini I, Di Rocco G, Ranieri A, Rosato A, Vanarotti M, Viezzoli MS, Vasos PR. 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]

**45**. Anastassopoulou J, Banci L, Bertini I, Cantini F, Katsari E, Rosato A. Solution structure of the apo-and copper(I) loaded human metallo-chaperone HAH1. Biochemistry, 43:13046-13053, 2004 [IF 3.922]

**46**. Bertini I, Rosato A. A genomic frontier in bioinorganic chemistry (Invited). Chem.Lett. 33:946-951, 2004 [IF 1.579] **47**. Banci L, Bertini I, Chasapis C, Ciofi-Baffoni S, Hadjiliadis N, 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]

**48**. Andreini C, Banci L, Bertini I, Elmi S, Rosato A. Comparative analysis of the ADAM and ADAMTS families. J. Proteome Res. 4:881-888, 2005 [IF 6.917]

**49**. Banci L, Bertini I, Cantini F, Chasapis C, Hadjiliadis N, Rosato, A. A NMR study of the interaction of a threedomain construct of ATP7A with copper(I) and copper(I)-HAH1: the interplay of domains. J. Biol. Chem. 280:38259-38263, 2005 [IF 6.355]

**50**. Banci L, Bertini I, Cantini F, Migliardi M, Rosato A, 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]

**51**. Bertini I, Cavallaro G, 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]

**52.** Andreini C, Banci L, Bertini I, Rosato, A. Counting the zinc proteins encoded in the human genome. J.Proteome Res. 5:196-201, 2006. [IF 6.901]

53. Bertini I, Cavallaro G, Rosato, A. Cytochrome c: occurrence and functions. Chem.Rev. 106:90-115, 2006 [IF 26.054]

**54**. Arnesano F, Banci L, Bertini I, Capozzi F, Ciurli S, Luchinat C, Mangani S, Ciofi-Baffoni S, Rosato A, Turano P, Viezzoli MS An Italian contribution to structural genomics: Understanding metalloproteins. (Invited Review). Coord.Chem.Rev. 250:1419-1450, 2006 [IF 9.779]

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#### Fact sheet

- Born in Florence, Italy on November 3<sup>rd</sup>, 1971
- Permanent researcher at the University of Florence from 1999 to 2002, then Associate Professor of Chemistry at the same University
- Co-Authored about 120 articles on peer-reviewed scientific journals of international renown (see <a href="http://scholar.google.ca/citations?user=oJGxsEoAAAAJ&hl=en">http://scholar.google.ca/citations?user=oJGxsEoAAAAJ&hl=en</a> or <a href="https://publons.com/researcher/M-3250-2019/">https://publons.com/researcher/M-3250-2019/</a>)
- Co-Authored 32 entries in the Protein Data Bank (<u>http://www.pdb.org</u>)
- H-index = 42, with more than 5000 citations (source: Web of Science)
- His research activity focuses on metalloproteins, i.e. proteins that bind metal ions to perform their biological function, and on high-resolution nuclear magnetic resonance, as a technique to investigate the 3D structure and the intermolecular interactions of proteins. He is especially active in the development and application of computational and bioinformatics methods.
- He was Scientific Manager of the e-NMR project, which created a distributed computing grid infrastructure involving the main NMR centers in Europe (http://www.e-nmr.eu), and was the P.I. of the Research unit at the University of Florence within the follow-up project WeNMR (http://www.wenmr.eu). The later project received an 'Excellent Science' prize awarded by the European Commission, in the "FP7 Success Story Competition". He is the P.I. of the Research unit at the University of Florence in various projects on the application of cloud computing to the analysis of scientific data in the Life Sciences.