

STEFANO CIURLI
Curriculum Vitae - Gennaio 2024

Institutional site: <https://www.unibo.it/sitoweb/stefano.ciurli>

Education:

October 1979 - December 1984

University of Pisa, Faculty of Sciences (Italy)

Chemistry Department

Major in Inorganic and Physical Chemistry

January 1985 - June 1986

Columbia University, New York, NY (USA)

Chemistry Department

Research Assistant – Tutor: Prof. Carlo Floriani

July 1986

University of Pisa, Faculty of Sciences (Italy)

Chemistry Department

Laurea 110/110 cum laude

"Synthesis, reactivity and structural characterization of metal complexes with macrocyclic ligands"

September 1986 – September 1990

Harvard University, Cambridge, MA (USA)

Chemistry Department

Ph.D. in Inorganic Chemistry – Tutor: Prof. Richard H. Holm

"Synthesis and properties of subsite-differentiated cubane clusters MFe_3S_4 "

September 1990 – September 1992

University of Bologna post-doctoral fellowship with Prof. Ivano Bertini and Prof. Claudio Luchinat

NMR spectroscopy and study of the electronic structure of iron-sulfur centers in proteins

Academic Career:

October 1992 – September 2001

University of Bologna

Associate Professor of Agricultural chemistry (AGR/07)

October 2001 - present

University of Bologna

Professor of General and Inorganic Chemistry (CHIM/03)

October 2004 - 2018

Free University of Bolzano

Professor of General and Inorganic Chemistry (CHIM/03)

January 2013 – December 2015

Universidade Federal do Rio Grande do Sul (Porto Alegre, Brazil) – Center for Biotechnology

Visiting Professor in the framework of the program Science without Borders (CAPES)

Academic Honors

Nominated by the Rector of the University of Bologna for the *excellent teaching quality in the course on Agricultural Biochemistry* (academic year 2002-2003)

Nominated by the Rector of the University of Bologna for the *excellent teaching quality in the course on General and Inorganic Chemistry* (academic year 2004-2005)

Member of the Istituto di Studi Avanzati, University of Bologna (2006-2012; 2019-2022)

Member of the Board of the Istituto di Studi Superiori - University of Bologna (2009-2012)

Tutor of the Collegio Superiore - University of Bologna (2016-present)

Lecturer for the following courses

Academic year	Course	Program
1992-1993	Soil fertility and plant nutrition	B.Sc. Agricultural Science
1993-1994	General and inorganic chemistry Chemistry and biochemistry of pesticides	B.Sc. Agricultural Science
1994-1995	Soil fertility and plant nutrition Chemistry and biochemistry of pesticides	B.Sc. Agricultural Science
1995-1996	Spectroscopic chemical analysis Chemistry and biochemistry of pesticides	B.Sc. Agricultural Science

1996-1997	Physical methods in inorganic chemistry Chemistry and biochemistry of pesticides	B.Sc. Agricultural Science
1997-1998	Agricultural biochemistry Chemistry and biochemistry of pesticides	B.Sc. Biotechnology
1998-1999	General and inorganic chemistry	B.Sc. Agricultural Science
1999-2000	Agricultural biochemistry General and inorganic chemistry Bioinorganic chemistry	B.Sc. Biotechnology B.Sc. Agricultural Science B.Sc. Biotechnology
2000-2001	Bioinorganic chemistry Agricultural biochemistry	B.Sc. Biotechnology B.Sc. Biotechnology
2001-2002	General and inorganic chemistry Agricultural biochemistry	B.Sc. Agricultural Science B.Sc. Biotechnology
2002-2003	General and inorganic chemistry Agricultural biochemistry	B.Sc. Agricultural Science B.Sc. Biotechnology
2003-2004	General and inorganic chemistry	B.Sc. Agricultural Science
2004-2005	General and inorganic chemistry Biomolecular NMR spectroscopy General and inorganic chemistry	B.Sc. Agricultural Science M.Sc. Molecular and Industrial Biotechnology B.Sc. Free University of Bolzano
2005-2006	General and inorganic chemistry Biomolecular NMR spectroscopy General and inorganic chemistry	B.Sc. Agricultural Science M.Sc. Molecular and Industrial Biotechnology B.Sc. Free University of Bolzano
2006-2007	General and inorganic chemistry Biomolecular NMR spectroscopy General and inorganic chemistry Water Chemistry	B.Sc. Agricultural Science M.Sc. Molecular and Industrial Biotechnology B.Sc. Free University of Bolzano M.Sc. Land and water conservation
2007-2008	General and inorganic chemistry Biomolecular NMR spectroscopy General and inorganic chemistry Water Chemistry	B.Sc. Agricultural Science M.Sc. Molecular and Industrial Biotechnology B.Sc. Free University of Bolzano M.Sc. Land and water conservation
2008-2013	General and inorganic chemistry Biomolecular NMR spectroscopy General and inorganic chemistry Water Chemistry	B.Sc. Agricultural Science M.Sc. Molecular and Industrial Biotechnology B.Sc. Free University of Bolzano M.Sc. in Land and water conservation
2013-2016	General and inorganic chemistry Biomolecular NMR spectroscopy General and inorganic chemistry General and inorganic chemistry	B.Sc. Agricultural Science M.Sc. Molecular and Industrial Biotechnology B.Sc. Free University of Bolzano M.Sc. Pharmaceutical Chemistry and Technology
2016-2018	General and inorganic chemistry General and inorganic chemistry Biomolecular NMR spectroscopy	M.Sc. Pharmaceutical Chemistry and Technology B.Sc. Free University of Bolzano M.Sc. Molecular and Industrial Biotechnology
2018-2023	General and inorganic chemistry Biomolecular NMR spectroscopy	M.Sc. Pharmaceutical Chemistry and Technology M.Sc. Molecular and Industrial Biotechnology

Course Content

The scope of the course in General Chemistry is to provide the basic knowledge of the structure of matter and thermodynamic and kinetic principles that govern its transformation, with particular attention to chemical reactions occurring in the environmental biosphere, through the study of structural and functional properties of small molecules involved in the cycles of nutrients. This description is built starting from the electronic structure of atoms and molecules, describing the nature of the chemical bond and the processes of its formation and breaking, also using

computational methods. The equilibria in homogeneous and heterogeneous phases are described with special focus on the treatment of acid-base and redox reactions. The course always includes a section on the role of metal ions in biological systems. The lectures in Bioinorganic chemistry, Agricultural Biochemistry and Soil Biochemistry contained references and concepts typical of the chemistry of metal ions in biological systems. The syllabus of Biomolecular Magnetic Resonance Spectroscopy involves the application of NMR spectroscopy to the structures of proteins and metallo-proteins in solution.

Tutor for the following Laurea Theses

- 1. Sofia Cei, Laurea in Scienze Agrarie**
Academic year 1995-1996
"Proteine Fe-S e citocromi coinvolte nel ciclo fotosintetico dei batteri *Rps. viridis* e *Rf. fermentans*. Caratterizzazione biochimica, spettroscopica, e funzionale"
- 2. Matteo Lamborghini, Laurea in Scienze Agrarie**
Academic year 1995-1996
"Proprietà biochimiche, spettroscopiche e funzionali di ureasi, citocromo c-553 e flavoemoproteina (FHP) isolate da un batterio alcalofilo del suolo, *Bacillus pasteurii*"
- 3. Silvia Miletto, Laurea in Scienze Agrarie**
Academic year 1995-1996
"Adsorbimento di ureasi su fosfati di calcio: un modello per l'idrolisi dell'urea nel suolo"
- 4. Afro Stecchezzi, Laurea in Chimica**
Academic year 1996-1997
"Studio del trasferimento elettronico foto-indotto in batteri fotosintetici implicati in processi ambientali biodegradativi"
- 5. Michela Marabini, Laurea in Scienze e Tecnologie Alimentari**
Academic year 1997-1998
"Spettroscopia SNIF-NMR applicata al settore agroalimentare"
- 6. Giuliano Sciara, Laurea in Scienze Biologiche**
Academic year 1998-1999
"Struttura in soluzione del citocromo c-553 ossidato da *Bacillus pasteurii* tramite spettroscopia NMR"
- 7. Massimo Strocchi, Laurea in Scienze Agrarie**
Academic year 1999-2000
"Purificazione del centro di reazione fotosintetico da *Chromatium vinosum*: studi cinetici di trasferimento elettronico fotoindotto utilizzando proteine mutate in siti specifici"
- 8. Massimiliano Stola, Laurea Magistrale in Biotecnologie Industriali**
Academic year 1999-2000
"Analisi teorica del meccanismo catalitico delle metallo-fosfatasi acide: implicazioni nel drug design"
- 9. Luca Lotito, Laurea Magistrale in Biotecnologie Industriali**
Academic year 1999-2000
"Espressione eterologa e purificazione di fosfatasi acida e UreG, proteine coinvolte nei cicli biochimici di fosforo e azoto"
- 10. Francesca Malerba, Laurea Magistrale in Biotecnologie Industriali**
Academic year 1999-2000
"Espressione eterologa, purificazione e caratterizzazione di una nichel-chaperonina: UreE da *Bacillus pasteurii*"

11. **Manuela Dezi, Laurea Magistrale in Biotecnologie Agrario-Vegetali**
Academic year 2001-2002
"Accumulo di cadmio in *Skeletonema costatum*: studi chimici e biochimici"
12. **Barbara Zambelli, Laurea Magistrale in Biotecnologie Industriali**
Academic year 2001-2002
"Espressione eterologa, purificazione, caratterizzazione e studi di modellistica molecolare di nichel-chaperonine"
13. **Giovanni Guarguaglini, Laurea Magistrale in Biotecnologie Agrario-Vegetali**
Academic year 2001-2002
"Isolamento e purificazione di una proteina responsabile dell'accumulo di Cd²⁺ in *Cylindrotheca fusiformis*"
14. **Cristina Baia, Laurea Magistrale in Biotecnologie Agrario-Vegetali**
Academic year 2002-2003
"UreD, una chaperonina coinvolta nell'introduzione del nichel nel sito attivo dell'ureasi"
15. **Stefano Torti, Laurea Magistrale in Biotecnologie Industriali**
Academic year 2003-2004
"Espressione, purificazione e cristallizzazione di UreE da *Bacillus pasteurii*: studi strutturali su una nichel-chaperonina"
16. **Matteo Savini, Laurea Magistrale in Biotecnologie Agrario-Vegetali**
Academic year 2004-2005
"UreG e UreD: approccio molecolare e computazionale per lo studio di proteine accessorie dell'ureasi"
17. **Marco Salomone, Laurea Magistrale in Scienze Biologiche**
Academic year 2004-2005
"Sulla biologia del nichel: un approccio biochimico e bioinformatico all'ureasi ed alle sue proteine accessorie"
18. **Matteo Bellucci, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2005-2006
"NikR di *Helicobacter pylori*: un regolatore trascrizionale nichel-dipendente"
19. **Fabio Martignani, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2006-2007
"Struttura e funzione di *Helicobacter pylori* UreG, una chaperonina nel metabolismo del nichel"
20. **Alice Soragni, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2006-2007
"Towards a structural characterization of Tau: Cu(II) toxic conformers"
21. **Rosanna Clima, Laurea in Scienze Biologiche**
Academic year 2008-2009
"Clonaggio ed espressione di UreD da *Helicobacter pylori*, una nichel-chaperonina dell'enzima ureasi"
22. **Andrea Raspadori, Laurea Magistrale in Biologia Molecolare e Cellulare**
Academic year 2009-2010
"Studi biochimici e strutturali di HypB da *Helicobacter pylori*: una metallo chaperonina della [Ni,Fe]-idrogenasi"
23. **Federico Agostini, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2009-2010
"Spettroscopia NMR di UreE da *Bacillus pasteurii*: struttura e dinamica di una nichel-chaperonina"
24. **Andrea Berardi, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2009-2010
"Espressione, purificazione e caratterizzazione di HpUreF: una metallo-chaperonina coinvolta nel meccanismo di attivazione e maturazione dell'ureasi di *H. pylori*"
25. **Luca Mazzei, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2010-2011
"Studi biochimici e strutturali su NikR da *Helicobacter pylori*, un regolatore trascrizionale nichel-dipendente"
26. **Cristian del Campo, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2010-2011

- "Studi biochimici e strutturali su Fur da *Helicobacter pylori*, un fattore di trascrizione ferro-dipendente"
- 27. Francesco Biagi, Laurea Magistrale in Biologia Molecolare e Cellulare**
Academic year 2011-2012
"Un approccio teorico-strutturale al metabolismo del nichel in *Helicobacter pylori*: modelli e interazioni proteina-proteina nell'attivazione di ureasi"
- 28. Manfredi Miraula, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2011-2012
"Struttura e funzione di UreG e RcnR, due proteine coinvolte nell'omeostasi e nel metabolismo del nichel nei batteri"
- 29. Cinzia Tarsia, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2012-2013
"Interazioni proteina-proteina in cellula: il trasporto del nichel nell'attivazione dell'ureasi di *Helicobacter pylori*"
- 30. Lucia Crisci, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2013-2014
"Espressione, purificazione e caratterizzazione di RcnR e Nur, regolatori dell'espressione genica dipendente da nichel"
- 31. Leonardo Bertini, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2014-2015
"Caratterizzazione cinetica e strutturale di vecchi e nuovi inibitori dell'ureasi"
- 32. Edoardo Salladini, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2014-2015
"Studi strutturali su Jaburetox, un insetticida naturale derivante dall'ureasi"
- 33. Francesca Benigni, Laurea Magistrale in Chimica e Tecnologie Farmaceutiche**
Academic year 2016-2017
"Caratterizzazione biochimica e strutturale dell'inibizione dell'ureasi: un enzima nichel - dipendente"
- 34. Umberto Contaldo, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2017-2018
"Inibizione dell'ureasi, un fattore di virulenza nichel dipendente. Caratterizzazione strutturale, biochimica e bioinformatica"
- 35. Elia Barchi, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2017-2018
"Studi strutturali sul repressore trascrizionale nichel-dipendente InrS di *Synechocystis sp.* pcc6803"
- 36. Andrea Dallapé, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2017-2018
"Characterization of a prebiotically plausible binuclear Iron-Sulfur Rieske-like cluster"
- 37. Elisa Evangelisti, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2018-2019
"Ammoniaca mono-ossigenasi: un approccio biotecnologico per migliorare l'efficienza della fertilizzazione azotata nel suolo"
- 38. Sebastiano Baldassar, Laurea Magistrale in Biotecnologie Molecolari e Industriali**
Academic year 2019-2020
"Studi strutturali sulla proteina DNA primasi umana"

Tutor for the following Ph.D. theses

- 1) **Silvia Miletto**
Doctorate in Crop production
University of Udine, 1997-1999
"Studio delle relazioni struttura-funzione dell'ureasi e delle proteine accessorie necessarie per l'assemblaggio del sito attivo contenente nichel"
- 2) **Massimiliano Stola**
Doctorate in Functional biology of cellular and molecular systems
University of Bologna, 2001-2003
"Caratterizzazione della metallo-chaperonina UreE: una proteina accessoria dell'ureasi"
- 3) **Barbara Zambelli**
Doctorate in Functional biology of cellular and molecular systems
University of Bologna, 2002-2005
"Caratterizzazione molecolare delle nichel-chaperonine UreG, UreF, e UreD: proteine proteina accessoria dell'ureasi"
- 4) **Matteo Bellucci**
Doctorate in Cellular, Molecular and Industrial Biology
University of Bologna, 2007-2009
"Molecular interactions: metal ions and protein chaperones in the urease system from *Helicobacter pylori*"
- 5) **Anna Merloni**
Doctorate in Cellular, Molecular and Industrial Biology
University of Bologna, 2011-2013
"Structural and biochemical studies of *Sporosarcina pasteurii* UreE: a nickel-chaperone involved in the urease activation process"
- 6) **Luca Mazzei**
Doctorate in Cellular, Molecular and Industrial Biology
University of Bologna, 2014-2016
"Structural and biochemical studies of urease: old and new inhibitors"

Other academic and research activities

- Coordinator of the ERASMUS/SOCRATES network in Agricultural Chemistry and Biochemistry with the Universities of Bologna, Kent, Rennes, Newcastle, Nottingham, Lleida, Cordova, Siviglia, Gottingen, Pisa (**1993-1998**)
- Board member of the research doctorate in "Crop productivity", University of Bologna and Udine (**1993-1999**)
- Board member of the Interuniversity Consortium on Magnetic Resonance of Paramagnetic Metallo-Proteins (CIRMMP), University of Firenze, Bologna and Siena (**1997-**)
- Board member of the Interdepartmental Consortium for Biotechnological Research (CIRB), University of Bologna (**1997-2012**)
- Board member of the Ph.D. program in "Functional biology of cellular and molecular systems", University of Bologna (**2000-2020**)
- Board member of the Ph.D. program in "Nanosciences for medicine and the environment", University of Bologna (**2021-**)
- Member of the Editorial Board of Chem. Tracts – Inorganic Chemistry (**2001-2003**)
Editor: Harry Gray, California Institute of Technology
- Elected Board member of the Council of the Division of Chemistry of Biological Systems of the Italian Chemical Society (**2000-2002** and **2012-2014**)
- Member of the Editorial Board of J. Biol. Inorg. Chem. (**2000-2002**)
- Member of the Editorial Board of J. Biol. Inorg. Chem. (**2004-2006**)
- Board member of the Institute for Advanced Studies, University of Bologna, **2007-2012; 2019-2021**
- Member of the evaluation committee of the Research School in "Metal Ions in Biological Systems – MIBS), Department of Life Sciences, University of Copenhagen – **2009**

- Member of the Editorial Board of J. Biol. Inorg. Chem. (2012–2014)
- Associate Editor for the Encyclopedia of Metalloproteins (Co, Ni, Cu), Springer (2010-2012)
- Member of the Editorial Board of PeerJ (2012-2014)
- Member of the Editorial Advisory Board of the Metallo-Biology book series (Royal Society of Chemistry) (2015-2016)
- Member of the Editorial Board of the Metallo-Biology book series (Royal Society of Chemistry) (2016-2021)
- Member of the Editorial Board of J. Biol. Inorg. Chem. (2019–2021)
- Director of the M.Sc. Program in Molecular and Industrial Biotechnology, University of Bologna (2015-2021)
- Guest Editor for the issue on “Nickel Biochemistry” of MDPI Inorganics (2019)
- Member of the Editorial Board of Journal of Inorganic Biochemistry (2020–2021)
- Guest Editor for the issue on “Nickel Biochemistry” of Inorganics (2019)
- Editorial Board Member for the International Journal of Molecular Sciences - Molecular Biophysics) (2019-2021)
- Editor in Chief for the “Journal of Inorganic Biochemistry” (Elsevier) (2022-)

Referee for international scientific journals:

J. Am. Chem. Soc.	Eur. J. Med. Chem.	FEBS Lett.	J. Biotechnol.
Biochemistry	Inorg. Chimica Acta	Int. J. Biol. Macromol.	J. Coll. Interf. Sci.
Eur. J. Inorg. Chem.	ChemBioChem	Inorg. Chem.	J. Mol. Biol.
J. Biol. Chem.	Biochimie	Acta Cryst.	J. Mol. Catal.
J. Biol. Inorg. Chem.	J. Inorg. Biochem.	Microbiology	Thermochim. Acta
Coord. Chem. Rev.	Arch. Biochem. Biophys.	Biochemical J.	J. Anal. Biochem.
Biochim. Biophys. Acta	Eur. J. Biochem.	J. Mol. Graph. Model.	ACS Med. Chem. Lett.
Biochem. Eng.	J. Mass Spectr.	J. Mol. Biol.	ChemCatChem
Bioorg. Chem.	J. Phys. Chem.	RSC Chem. Commun.	
Comp. Biol. Med.	J. Mol. Evol.	J. Bacteriol.	

Research Interests:

The main interest of my research activity is the elucidation of the role of metals found in biomolecules. The final goal is the identification of the molecular structure of the active site of metallo-enzymes, and the elucidation of structure-function relationships. The objective is to determine how the chemistry of the metal ion is modulated by the protein matrix, and thus to determine the mode of interaction with the substrate or with other proteins.

Proteins from bacteria living in waters and soils are purified, and their biochemical characterization is performed. Then, by applying sophisticated physical methods such as mono- and multidimensional NMR spectroscopy, EPR, Mössbauer, circular dichroism, magnetic susceptibility, bioelectrochemistry, X-ray spectroscopy (EXAFS), Raman and crystallography the structure of the active site is elucidated at the molecular level. Subsequently, mechanistic studies of the protein-substrate or protein-protein interactions are carried out using classic kinetic measurements or, for the photosynthesis-related projects, laser-induced rapid transient kinetics. Molecular mechanics and dynamics are used to model protein-substrate and protein-protein interactions.

In particular, on-going research projects involve i) biochemistry of metallo-enzymes involved in the nitrogen, phosphorous and sulfur cycles in the environment, ii) biochemistry of photosynthesis.

Research grants:

1993 – 1997 (L. 55,000,000)

National Research Council (CNR): "Indagine sulla relazione struttura-funzione dell'ureasi, un enzima del suolo importante per la nutrizione delle piante: utilizzo di tecnologie avanzate per lo studio dell'interazione enzima-inibitori"

1997 – 1999 (L. 210,000,000)

Contract NMR with Ministero delle Politiche Agricole

"Applicazione del metodo SNIF-NMR per la determinazione del rapporto isotopico $^2\text{D}/^1\text{H}$ in matrici biologiche"

1997 – 1999 (L. 335,000,000)

Research program of national interest – PRIN

"NMR di metallo-biomolecole paramagnetiche".

1997-2000 (L. 40,000,000)

NATO Linkage Grant

"Molecular Studies on Photosynthetic Redox Proteins Alternative to Cytochromes c_2 "

1998 -2000 (L. 260,000,000)

European Project Biotech-II

"Iron Containing Phosphatases: Structure and Function"

1998-2001 (L. 7,000,000)

European Project INTAS

"Biomimetic model complexes for dinuclear active sites of metalloproteins"

1999 -2000 (L. 244,000,000)

Research program of national interest – PRIN

"Il ruolo del cofattore metallico nella biologia strutturale inorganica"

2001-2005 (€ 7,500)

European Project Marie Curie Training Site

"Metals in biological systems"

2001-2003 (€ 22,500)

NATO Linkage Grant

"The development of biosensor technology for monitoring antioxidant activity of beverages"

2001 - 2003 (€ 90,000)

European Project INTAS

" Monitoring of total antioxidant activity in different beverages using biosensors technology "

2002 - 2004 (€ 81,000)

European Project INTAS

"EPR and electrometric study of the photosynthetic pigment-protein complexes in chloroplasts and hybrid model systems"

2001 - 2003 (€ 116,200)

Research program of national interest – PRIN

"Biologia strutturale inorganica nell'era post-genomica: metodologie e targeting".

2003 - 2005 (€ 55,800)

Research program of national interest – PRIN

"Il ruolo degli ioni metallici nei processi metabolici"

2005 - 2007 (€ 48,000)

Research program of national interest – PRIN

"Genomica strutturale di metalloproteine e delle loro interazioni funzionali"

2006 - 2007 (€ 45,000)

Progetto Strategico UniBO – in collaborazione con il Prof. Vincenzo Scarlato

" Molecular mechanisms governing essential urease and hydrogenase activity in the human gastric pathogen *Helicobacter pylori* "

2007 - 2009 (€ 37,000)

Research program of national interest – PRIN

"Gli ioni metallici nelle interazioni proteina-proteina"

2009 - 2011 (€ 16,000)

Research program of national interest – PRIN

"Biologia strutturale meccanicistica: avanzamenti metodologici e biologici"

2010 - 2014 (€ 425,000)

Research grant from Specialty Fertilizer Products LLC (USA)

"The role of polysaccharides in the efficiency of soil nitrogen fertilization with urea".

2013-2015 (€ 55,400)

Research program Science without borders – CAPES Foundation, Government of Brazil

"Estrutura tridimensional e potencial biotecnológico de peptídeos derivados de ureases"

2016-2023 (€ 380,000)

Research grants from Verdesian LLC (USA)

Membership of societies:

American Chemical Society

Italian Chemical Society

Society of Bio-Inorganic Chemistry

Biochemical Society

International Biometals Society

Harvard Club of Italy

Invited speaker at National Academic Institutions

- University of Firenze, Department of Chemistry, December **1989**
- University of Udine, Department of Plant Production, October **1994**
- University of Firenze, Department of Chemistry, May **1997**
- University of Udine, Department of Plant Production, May **1997**
- International School for Advanced Studies, Trieste, February **1998**
- University of Pisa, Department of Chemistry, April **2002**
- University of Bologna, Department of Agro-Environmental Science and Technology, February **2004**
- University of Bologna, Department of Agronomy, June **2004**
- University of Bologna, Department of Pharmacy and Biotechnology, November **2012**
- University of Trento, Centre for Integrative Biology, February **2014**
- Free University of Bolzano, June **2018**

Invited speaker at Foreign Academic Institutions

- University di Hamburg (Germany), Department of Chemistry, April **1991**
- New College of the University of South Florida (USA) April **1995**
- University of California Santa Cruz (USA) Department of Chemistry, April **1996**
- University of Lund (Sweden), Department of Inorganic Chemistry, September **1996**
- University of Copenhagen (Denmark) Department of Chemistry, September **1996**
- University of Lund (Sweden), Department of Inorganic Chemistry, August **1997**
- European Molecular Biology Laboratory, Hamburg Outstation (Germany) January **1997**
- Università di Hamburg, (Germany) Department of Chemistry, June **1999**
- Università di Gent, (Belgium) Department of Protein Biochemistry, February **2003**
- Moscow State University, (Russia) Department of Biological Chemistry, February **2003**
- University of Trondheim (Norway), Department of Biotechnology, July **2005**
- University of Lund (Sweden), Department of Chemical Physics, June **2006**
- Dartmouth College (USA), Department of Chemistry, April **2008**
- University of Lund (Sweden), Department of Chemistry, November **2008**
- University of Trondheim (Norway), Department of Biotechnology, June **2009**
- German Research School for Simulation Sciences GmbH, Jülich (Germany) July **2010**
- University of Massachusetts at Amherst (USA), Department of Chemistry, March **2011**
- Universidade Federal do Rio Grande do Sul, Center for Biotechnology, Porto Alegre (Brazil), January **2013**
- University Federal do Rio de Janeiro, Medical Biochemistry Institute, Rio de Janeiro (Brazil), June **2013**
- Pontificia Universidade Católica do Rio Grande do Sul, Instituto do Cérebro, Porto Alegre (Brazil), Sept. **2014**
- Universidade de Brasília, Brasília (Brazil), January **2015**
- University of South Florida, Department of Molecular Medicine, Tampa, FL (USA), March **2015**
- European Molecular Biology Laboratory c/o DESY, Hamburg (Germany), July **2015**
- University of Melbourne, School of Chemistry, Melbourne (Australia), October **2016**
- University of Queensland, School of Chemistry and Molecular Biosciences, Brisbane (Australia), November **2016**
- Institute Pasteur, Department of Structural Biology and Biochemistry, Paris (France), October **2018**
- Rensselaer Polytechnical Institute, Troy (NY, USA), February **2021**

Invited speaker at National Scientific Meetings

- National Congress of the Agricultural Chemistry Society (SICA), Piacenza, September **1994**
- National Congress of the Interdivisional Group of Magnetic Resonance of the Italian Chemical Society, Rimini, October **1996**
- Division of Chemistry of Biological Systems, Italian Chemical Society meeting, Parma, December **1997**
- Division of Inorganic Chemistry, Italian Chemical Society meeting, Maratea, June **1998**
- Division of Chemistry of Biological Systems, Italian Chemical Society meeting, Rimini, June **2000**
- School for Ph.D. students in Inorganic Chemistry "Bioinorganic Chemistry", S. Miniato, June **2002**
- Magnetic Resonance Group, Italian Chemical Society meeting, Porto Conte, September **2004**
- National Congress of the Italian Society of Biochemistry, Riccione, September **2005**
- Division of Chemistry of Biological Systems, Italian Chemical Society meeting, Sorrento, July **2009**
- Ph.D School in Bioinorganic Chemistry, Pontignano, Siena (Italy), July **2011**
- Division of Inorganic Chemistry, Italian Chemical Society meeting, Lecce, September **2011**

Invited speaker at International Scientific Meetings

- Workshop on Transition Metal Clusters in Biology, Medizinische Universität, Lubeca, Germany, April **1991**
- American Chemical Society Congress, Denver (USA), April **1993**
- 3rd Greek-Italian-Portuguese-Spanish Meeting in Inorganic Chemistry, Senigallia, June **1995**
- NATO Advanced Research Workshop "New Trends In Biosensor Development" Kiev, Ukraine, March **1998**
- XXXIII International Conference Coordination Chemistry (ICCC) Firenze, August **1998**
- 2nd International Workshop on "Structural Characterization of Proteins by NMR, X-Ray Diffraction, and Computational Methods", University of Verona, February **1999**
- 5th International Symposium on Applied Bioinorganic Chemistry Corfu, Greece, April **1999**
- 9th International Conference of Bioinorganic Chemistry (ICBIC-9), Minneapolis (USA), June **1999**.
- Symposium on Bioinorganic Chemistry, Chemical Center, University of Lund, June **2000**.
- Biotechnology Winter School on Biomolecular Docking in Silico, Bologna, February **2001**
- 20th European Crystallographic Meeting (ECM20) Krakow, Poland, August **2001**
- 3rd International Workshop on "Structural Characterization of Proteins by NMR, X-Ray Diffraction, and Computational Methods", S. Vito di Cadore, Italy, September **2001**
- Indo-Italian meeting on "NMR of Biological Systems" Lucknow, India, January **2002**
- Meeting on Metal in Biology, Autrans/Grenoble, France, March **2002**
- 6th European Conference on Bioinorganic Chemistry (EUROBIC-6), Copenhagen/Lund, July **2002**
- 7th FIGIPS, Meeting in Inorganic Chemistry, Lisbon (Portugal) June **2003**

- 11th International Conference of Bioinorganic Chemistry (ICBIC-11), Cairns (Australia), July **2003**
- COST meeting D21 on Metalloenzymes and chemical biomimetics, Thessaloniki (Greece), September **2003**
- 1st International Meeting on Metal Homeostasis, Institute of Metals in Biology of Grenoble, Villard de Lans (France), September **2004**
- COST meeting D21 on Metalloenzymes and chemical biomimetics, Rome (Italy), May **2005**
- International Conference on Biocatalysis, Nordforsk Research Training Course on High-Speed NMR Protein Structure Analysis, Moscow - S. Petersburg (Russia), June **2007**
- 13th International Conference of Bioinorganic Chemistry (ICBIC-13), Vienna (Austria), July **2007**.
- 235th Congress of the American Chemical Society, New Orleans (USA), April **2008**.
- Graduate Summer School in Metal Ions in Biological Systems, Holbæk (Denmark), June **2008**
- 9th European Conference on Bioinorganic Chemistry (EUROBIC-9), Wroklaw, (Poland), September **2008**
- 237th Congress of the American Chemical Society, Salt Lake City (USA), March **2009**
- NordForsk Research Course on "Macromolecular Interactions – Biology and Emerging Tools, Riccione (Italy) September **2009**.
- 239th Congress of the American Chemical Society, San Francisco (USA), March **2010**
- 240th Congress of the American Chemical Society, Boston (USA), August **2010**
- 241th Congress of the American Chemical Society, Anaheim (USA), March **2011**
- 15th International Conference of Bioinorganic Chemistry (ICBIC-15), Vancouver (Canada), August **2011**.
- 243th Congress of the American Chemical Society, San Diego (USA), March **2012**
- 245th Congress of the American Chemical Society, New Orleans (USA), April **2013**
- Zing Conference on Bioinorganic Chemistry, Lanzarote (Spain), February **2013**
- 16th International Conference of Bioinorganic Chemistry (ICBIC-16), Grenoble (France), July **2013**.
- 248th Congress of the American Chemical Society, Denver (USA), March **2015**
- 23rd Congress of the International Union of Biochemistry and Molecular Biology (IUBMB), Foz do Iguacu (Brazil), August **2015**
- 17th International Biotechnology Symposium, Melbourne (Australia), October **2016**
- 253rd Congress of the American Chemical Society, San Francisco (USA), April **2017**
- 18th International Conference of Bioinorganic Chemistry (ICBIC-18), Florianopolis (Brazil), July **2017**
- International Annual Meeting of the American Society of Agronomy, Crop Science Society of America, and Soil Science Society of America, Tampa (USA), October **2017**
- 18th Biotechnology Congress, New York (USA), October **2017**
- 7th Intern. Conference on the Development of Biomedical Engineering, Ho Chi Minh City (Vietnam), June **2018**.
- Summer Annual Meeting of AAPFCO (Association of American Plant Food Control Officials), Ft. Lauderdale (FL, USA), August **2018**.
- 19th International Conference of Bioinorganic Chemistry (ICBIC-19), Interlaken (Switzerland), July **2019**.
- 12th International Biometals Symposium – BioMetals 2020, Grenoble (France), July **2020**.
- Canadian Chemistry Conference and Exhibition, Calgary (Canada), June **2022**.
- 16th European Conference on Bioinorganic Chemistry (EUROBIC-16), Grenoble (France), July **2022**
- Gordon Research Conference on Metal Ions in Biology, Ventura (CA, USA), January **2023**
- 8th Canadian Conference on Bioinorganic Chemistry (CanBIC-8), Perry Sound (ON, Canada), May **2023**
- 16th International Symposium on Applied Bioinorganic Chemistry (ISABC-16), Ioannina (Greece), June **2023**

Research Experience

My research curriculum reflects an evolution from basic coordination and organometallic chemistry to model bio-inorganic chemistry, and finally to inorganic biochemistry. This evolution has allowed me to build on chemical grounds a level and breadth of knowledge extremely useful to understand the role of metals in biological processes. Furthermore, the application of a large variety of physical methods to model compounds has been a learning bench for further applications of the same techniques to more complex biomolecules. I believe that a complementary role of both model chemistry and biochemistry is fundamental for the understanding of the interaction of bio-molecules with metal ions.

1985-1986

Functionalization of late transition metal (Fe, Co, Ni, Cu) porphyrino-type complexes, with the goal of study low oxidation states of the metals in ionic pair form with alkali ions. Synthesis of complexes between early transition metals (Ti, Zr, V, Nb) and highly sterically flexible macrocycles to obtain cis-coordination sites possibly available for catalysis. The techniques used involved Schlenk-line manipulation of highly air-sensitive compounds. Instrumentation used included IR, UV-vis, and 1D ^1H and ^{13}C NMR spectroscopies. Some knowledge of X-ray crystallography of small molecules was also gained.

1986-1990

Synthesis of metal-sulfur clusters as models for metallo-proteins and metallo-enzymes. The properties of subsite-differentiated cubane-type clusters of the type MFe_3S_4 (M=Fe, V, Mo, Re, Co, and Ni) were investigated. In the case of M=Fe, subsite differentiation was achieved by the use of a complex organic ligand, binding the cluster to three Fe sites and leaving the fourth Fe ion available for modulation of reactivity, and of structural and spectroscopic properties significant for the biological involvement of the Fe_4S_4 cluster in enzymatic catalysis. In the case of V and Mo, the reactivity of the heteroatom in the cluster was studied spectroscopically. In the case of Re, Ni, and Co, new routes for the synthesis of the corresponding heteroatom cluster were developed, and the structures and properties of the resulting complexes were studied both spectroscopically and using X-ray crystallography. The techniques used involved Schlenk-line and dry-boxes manipulation of air-sensitive compounds, organic synthesis, UV-vis spectroscopy, 1D and 2D NMR spectroscopy, electrochemistry (cyclic voltammetry, differential pulse polarography, coulometry), X-ray crystallography, Mossbauer spectroscopy, EPR spectroscopy, magnetic susceptibility measurements using NMR and SQUID. Acquaintance with EXAFS spectroscopy was also gained.

1990-1992

NMR spectroscopy of iron-sulfur proteins. Relationships between structural and magnetic, Mossbauer, NMR, and EPR spectroscopic parameters in iron-sulfur proteins. Theoretical models of magnetic exchange. Molecular mechanics and dynamics of iron-sulfur proteins. Relationships between structure and redox potential in iron-sulfur proteins.

1992-present

Isolation, purification, and physical characterization of soluble and membrane-bound proteins involved in bacterial photosynthesis. Studies of electron-transfer processes between soluble and membrane-bound electron carriers using rapid light-induced time-resolved kinetic spectrophotometry.

Isolation, purification, and physical characterization of bacterial nickel proteins. Structural studies using XAS spectroscopy. Protein crystallization and X-ray structure determination of bacterial urease. Applications of high resolution nuclear magnetic resonance (NMR) spectroscopy to the determination of the structure of metallo-biomolecule.

Molecular mechanics and dynamics of metallo-biomolecules.

Computer assisted rational drug design of inhibitors for metallo-enzymes.

Structural biology and biochemistry of nickel trafficking proteins.

Nickel-dependent transcription factors in soil and pathogenic bacteria.

Research activities abroad

<u>March 1995</u>	Department of Biochemistry, University of Tucson, Arizona (USA)
<u>June-August 1995</u>	New College of the University of South Florida, Division of Natural Sciences (USA)
<u>November 1995</u>	European Molecular Biology Laboratory, Heidelberg (Germany)
<u>June-August 1997</u>	Department of Inorganic Chemistry, Lund University (Sweden)
<u>June 1999</u>	European Molecular Biology Laboratory, Hamburg (Germany)
<u>June-July 2006</u>	Department of Inorganic Chemistry, Lund University (Sweden)
<u>June 2009</u>	Department of Biotechnology, University of Science and Technology, Trondheim (Norway)
<u>Jan. 2013-Dec. 2015</u>	Center for Biotechnology, Universidade Federal do Rio Grande do Sul, Porto Alegre (Brazil)
<u>June 2022</u>	Rensselaer Polytechnic Institute (RPI) - Troy (NY, USA)

STEFANO CIURLI

Publication list – September 2023

Scholar: <http://scholar.google.com/citations?user=i2O2sokAAAAJ&hl=en>ORCID: <http://orcid.org/0000-0001-9557-926X>ResearcherID: <http://www.researcherid.com/rid/K-4355-2014>

Scopus Author ID: 7003777670

Impact factors from ISI for each corresponding year, when available

Paper on Bismuth with Braga-Grepioni

Paper on CryoEM with Cianci-Tria

Paper on Origin of Life with Mansy

Paper on ITC and Mpro with Montelione

Paper on PLpro with Montelione

#187 J. A. Hernandez; P. Micus; S. A. L. Sunga; L. Mazzei; S. Ciurli; G. Meloni*

"Metal selectivity and translocation mechanism characterization in proteoliposomes of the transmembrane NiCoT transporter NixA from *Helicobacter pylori*"**2023** – Accepted for publication in *Chem. Sci.*

#186 N. Carosella; K. Brock; B. Zambelli; F. Musiani; C. Sander; S. Ciurli*

"Functional contacts for activation of urease from *Helicobacter pylori*: an integrated approach using evolutionary couplings, in-cell enzymatic assays, and computational docking"*Front. Chem. Biol.* **2023**, 2 (doi: 10.3389/fchbi.2023.1243564)

#185 L. Mazzei; * A. Paul; M. Cianci; M. Devodier; D. Mandelli; P. Carloni; S. Ciurli

"Kinetic and structural details of urease inactivation by thiuram disulphides"

2023, *J. Inorg. Biochem.*

#184 L. Mazzei; F. Musiani; B. Zambelli; S. Benini; M. Cianci; S. Ciurli*

"Urease: structure, function, catalysis, and inhibition" (Ed. Elsevier)

2023, In press#183 K. Macegoniuk; W. Tabor; L. Mazzei; M. Cianci; M. Giurg; K. Olech; M. Burda-Grabowska; R. Kaleta; A. Grabowiecka; A. Mucha; S. Ciurli; Ł. Berlicki*

"Optimized ebselen-based inhibitors of bacterial ureases with nontypical mode of action"

J. Med. Chem. **2023**, 66, 2054-2063

#182 L. Mazzei; R. Greene-Cramer; K. Bafna; A. Jovanovic; A. De Falco; T. B. Acton; C. A. Royer; S. Ciurli*; G. T. Montelione"

"Protocol for production and purification of SARS-CoV-2 3CLpro"

Cell STAR Protocols **2023**, 4, 102326#181 B. Zambelli; P. Basak; H. Hu; M. Piccioli; F. Musiani; V. Broll; L. Imbert; J. Boisbouvier; M. Maroney*; S. Ciurli*"The structure of the high-affinity nickel-binding site in the Ni,Zn-HypA•UreE₂ complex"*Metallomics* **2023**, 15, mfad003#180 Y. Beniamino; V. Cenni; S. Ciurli*; B. Zambelli*

"The nickel binding activity of the intrinsically disordered region of human NDRG-1, a protein involved in cancer development"

Biomolecules, **2022**, 12, 1272-1298

IF: 6.064 – Q2 – Biochemistry and Molecular Biology

#179 L. Mazzei*; M. Cianci; S. Ciurli

"Inhibition of urease by hydroquinones: a structural and kinetic study"

Chem. Eur. J. **2022**, 28, e202201770

IF: 5.020 – Q2 – Chemistry Multidisciplinary

#178 L. Casali; L. Mazzei; R. Sun; M. R. Chierotti; R. Gobetto*; D. Braga; F. Grepioni*; S. Ciurli*

"Thiocarbamoyl disulfides as inhibitors of urease and ammonia monooxygenase: crystal engineering towards enhanced nitrogen soil fertilization"

Crystal Growth & Design, **2022**, 22, 4528-4537

IF: 4.010 – Q1 – Crystallography

- #177 P. Basak; B. Zambelli; D. E. Cabelli; [S. Ciurli](#); M. J. Maroney*
 "Pro5 is not essential for the formation of 'Ni-Hook' in Nickel Superoxide Dismutase"
J. Inorg. Biochem. **2022**, 234, 111858
 IF: 4.336 – Q1 – Chemistry, Inorganic & Nuclear
- #176 L. Mazzei; F. Musiani; S. Szerko; V. Kozminski; M. Cianci; Y. Beniamino; [S. Ciurli](#);* B. Zambelli*
 "Structure, dynamics and function of SrnR, a transcription factor for nickel-dependent gene expression"
Metalomics **2021**, 13, mfab069
 IF: 4.636 – Q2 – Biochemistry & Molecular Biology
- #175 G. Camporesi; A. Minzoni; L. Morasso; [S. Ciurli](#)*; F. Musiani*
 "Nickel import and export in the human pathogen *Helicobacter pylori*, perspectives from molecular modelling"
 Zambelli, B; Basak, P; Hu, H; Piccioli, M; Musiani, F; Broll, V; Imbert, L; Boisbouvier, J; Maroney, MJ; Ciurli, S"
Metalomics **2021**, 13, mfab066
 IF: 4.636 – Q2 – Biochemistry & Molecular Biology
- #174 L. Mazzei*; L. Massai; M. Cianci; L. Messori; [S. Ciurli](#)*
 "Medicinal Au(I) compounds targeting urease as prospective antimicrobial agents: unveiling the structural basis for enzyme inhibition"
Dalton Trans. **2021**, 50, 14444-14452
 IF: 4.569 – Q1 – Chemistry, Inorganic & Nuclear
- #173 L. Casali; V. Broll, [S. Ciurli](#)*; F. Emmerling, D. Braga; F. Grepioni*
 "Facilitating nitrification inhibition through green, mechanochemical synthesis of a novel nitrapyrin complex"
Crystal Growth & Design, **2021**, 21, 5792-5799
 IF: 4.010 – Q1 – Crystallography
- #172 E. Darrouzet; C. Rinaldi; B. Zambelli; [S. Ciurli](#); C. Cavazza*
 "Revisiting the CooJ family, a potential chaperone for nickel delivery to [NiFe]-carbon monoxide dehydrogenase"
J. Inorg. Biochem. **2021**, 225, 111588
 IF: 4.336 – Q1 – Chemistry, Inorganic & Nuclear
- #171 M. Masetti*; M. Bertazzo; M. Recanatini; [S. Ciurli](#); F. Musiani*
 "Probing the transport of nickel ions through the internal tunnels of the *HpUreDFG* multimeric complex"
J. Inorg. Biochem. **2021**, 223, 111554
 IF: 4.336 – Q1 – Chemistry, Inorganic & Nuclear
- #170 L. Mazzei; [S. Ciurli](#)*
 "Urease"
Encyclopedia of Inorganic and Bioinorganic Chemistry (A. Messerschmidt Ed.); John Wiley & Sons, Ltd, Chichester (UK), **2021**, pp. 1-17 (DOI: 10.1002/9781119951438.eibc2776)
- #169 M. J. Maroney*; [S. Ciurli](#)
 "Nickel as a virulence factor in the class I bacterial carcinogen, *Helicobacter pylori*"
Semin. Cancer Biol. **2021**, 76, 143-155
 IF: 17.012 – Q1 – Oncology
- #168 L. Mazzei*; D. Cirri; M. Cianci; L. Messori; [S. Ciurli](#)*
 "Kinetic and structural analysis of the inactivation of urease by mixed-ligand phosphine halide Ag(I) complexes"
J. Inorg. Biochem. **2021**, 218, 111375
 IF: 4.336 – Q1 – Chemistry, Inorganic & Nuclear
- #167 L. Mazzei*; U. Contaldo; F. Musiani; M. Cianci; G. Bagnolini; M. Roberti; [S. Ciurli](#)*
 "Inhibition of urease, a Ni-enzyme: the reactivity of a key thiol with mono- and di-substituted catechols elucidated by kinetic, structural and theoretical studies"
Angew. Chem. Int. Ed. **2021**, 60, 6029-6035
 IF: 16.823 – Q1 – Chemistry Multidisciplinary
- #166 F. Musiani;* V. Broll; E. Evangelisti; [S. Ciurli](#)*
 "The model structure of the copper-dependent ammonia monooxygenase"
J. Biol. Inorg. Chem. **2020**, 25, 995-1007
 IF: 3.358 – Q2 – Chemistry, Inorganic & Nuclear
- #165 L. Mazzei; F. Musiani; [S. Ciurli](#)*

"The structure-based reaction mechanism of urease, a nickel dependent enzyme: tale of a long debate"

J. Biol. Inorg. Chem. **2020**, *25*, 829-845

IF: 3.358 – Q2 – Chemistry, Inorganic & Nuclear

#164 A. Pierro; E. Etienne; G. Gerbaud; B. Guigliarelli; S. Ciurli; V. Belle; B. Zambelli*; E. Mileo*

"Nickel and GTP modulate *Helicobacter pylori* UreG structural flexibility"

Biomolecules, **2020**, *10*, 1062-1079

IF: 4.879 – Q2 - Biochemistry & Molecular Biology

#163 M. Masetti; F. Falchi; D. Gioia; M. Recanatini; S. Ciurli; F. Musiani*

"Targeting the protein tunnels of the urease accessory complex: a theoretical investigation"

Molecules **2020**, *25*, 2911

IF: 4.412 – Q2 – Biochemistry & Molecular Biology

#162 B. Zambelli*; L. Mazzei; S. Ciurli

"Intrinsic disorder in the nickel-dependent urease network"

Prog. Mol. Biol. Transl. **2020**, *1*, 307-330

IF: 3.622 – Q3 - Biochemistry & Molecular Biology

#161 M. J. Maroney*; S. Ciurli*

"Bioinorganic chemistry of nickel – Editorial"

Inorganics **2019**, *7*, 131-132

#160 K. Kappaun; A. H. S. Martinelli; V. Broll; B. Zambelli; F. C. Lopes; R. Ligabue-Braun; L. L. Fruttero; N. R. Moyetta; C. D. Bonan; C. R. Carlini*; S. Ciurli*

"Soyuretox, an intrinsically disordered polypeptide derived from soybean (*Glycine max*) ubiquitous urease with potential use as a biopesticide"

Int. J. Mol. Sci. **2019**, *20*, 5401-5420

I.F. 4.556 – Q1 – Biochemistry & Molecular Biology

#159 M. Alfano; G. Veronesi; F. Musiani; B. Zambelli; L. Signor; O. Proux; M. Rovezzi; S. Ciurli*; C. Cavazza*

"A solvent-exposed cysteine forms a novel Ni(II)-binding site in the metallochaperone CooT from *Rhodospirillum rubrum*"

Chem. Eur. J. **2019**, *25*, 15351 – 15360

I.F. 4.857 – Q1 – Chemistry, Multidisciplinary

#158 C. Samori*; L. Mazzei; S. Ciurli; G. Cravotto; G. Grillo; E. Guidi; A. Pasteris; S. Tabasso; P. Galletti

"Urease Inhibitory Potential and Soil Ecotoxicity of Novel "Polyphenols–Deep Eutectic Solvents" Formulations"

ACS Sus. Chem. Eng. **2019**, *7*, 15558-15567

I.F. 7.632 – Q1 – Chemistry Multidisciplinary

#157 L. Mazzei; M. Cianci; S. Benini; S. Ciurli*

"The impact of pH on catalytically critical protein conformational changes: the case of the urease, a nickel enzyme"

Chem. Eur. J. **2019**, *25*, 12145-12158

I.F. 4.857 – Q1 – Chemistry, Multidisciplinary

#156 L. Mazzei; V. Broll; L. Casali; M. Silva; D. Braga; F. Grepioni*; J. Baltrusaitis*; S. Ciurli*

"Multifunctional urea cocrystal with combined ureolysis and nitrification inhibiting capabilities for enhanced nitrogen management"

ACS Sus. Chem. Eng. **2019**, *7*, 13369 - 13378

I.F. 7.632 – Q1 – Chemistry Multidisciplinary

#155 L. Mazzei; M. Cianci; S. Benini; S. Ciurli*

"The structure of the elusive urease-urea complex unveils the mechanism of a paradigmatic nickel-dependent enzyme"

Angew. Chem. Int. Ed. **2019** *131*, 7493-7497

IF: 12.959 – Q1 – Chemistry Multidisciplinary

#154 M. Alfano; J. Pérard; P. Carpentier; C. Bassett; B. Zambelli; J. Timm; S. Crouzy; S. Ciurli; C. Cavazza*

"The carbon monoxide dehydrogenase accessory protein CooJ is a histidine-rich multidomain dimer containing an unexpected Ni(II)-binding site"

J. Biol. Chem. **2019**, *294*, 7601-7614

IF: 4.238 – Q2 – Biochemistry & Molecular Biology

#153 L. Mazzei; M. N. Wenzel; M. Cianci; M. Palombo; A. Casini*; S. Ciurli*

"Inhibition mechanism of urease by Au(III) compounds unveiled by X-ray diffraction analysis"

ACS Med. Chem. Lett. **2019**, *10*, 564-570

IF: 3.975 – Q2 – Chemistry, Medicinal

#152 L. Mazzei; M. Cianci; U. Contaldo; S. Ciurli*

"Insights into urease inhibition by N-(n-butyl) phosphoric triamide through an integrated structural and kinetic approach"

J. Agric. Food Chem. **2019**, *67*, 2127-2138

IF: 4.192 – Q1 – Chemistry Applied

#151 L. Casali; L. Mazzei; O. Shemchuk; L. Sharma; K. Honer; F. Grepioni*; S. Ciurli*; D. Braga; J. Baltrusaitis*
"Novel dual-action plant fertilizer and urease inhibitor: the urea-catechol co-crystal - characterization and environmental reactivity"

ACS Sustain. Chem. Eng. **2019**, *7*, 2852-2859

I.F. 7.632 – Q1 – Chemistry, Multidisciplinary

#150 C. A. E. M. Spronk; S. Žerko; M. Górka; W. Koźmiński; B. Bardiaux; B. Zambelli; F. Musiani; M. Piccioli; P. Basak; F. C. Blum; R. C. Johnson; H. Hu; D. S. Merrell; M. J. Maroney*; S. Ciurli*

"Structure and dynamics of *Helicobacter pylori* nickel-chaperone HypA: an integrated approach using NMR spectroscopy, functional assays and computational tools"

J. Biol. Inorg. Chem., **2018**, *23*, 1309-1330

IF: 2.952

#149 C. Tarsia; A. Danielli; F. Florini; P. Cinelli; S. Ciurli; B. Zambelli*

"Targeting *Helicobacter pylori* urease activity and maturation: in-cell high-throughput approach for drug-discovery"

BBA – Gen. Subj., **2018**, *1862*, 2245-2253

IF: 3.679

#148 L. Casali; L. Mazzei; O. Shemchuk; K. Honer; F. Grepioni*; S. Ciurli*; D. Braga; J. Baltrusaitis*

"Smart urea ionic cocrystals with enhanced urease inhibition activity for improved nitrogen cycle management"

Chem. Commun. **2018**, *54*, 7637-7640

IF: 6.164

#147 L. Mazzei; M. Cianci; A. G. Vara; S. Ciurli*

"The structure of urease inactivated by Ag(I): a new paradigm for enzyme inhibition by heavy metals"

Dalton Trans. **2018**, *47*, 8240-8247

IF: 4.052

#146 L. Mazzei; V. Broll; S. Ciurli*

"An evaluation of maleic-itaconic copolymers as urease inhibitors"

Soil Sci. Soc. Am. J. **2018**, *82*, 994-1003

IF: 1.997

#145 L. Mazzei; M. Cianci; U. Contaldo; F. Musiani; S. Ciurli*

"Urease inhibition in the presence of N-(n-butyl)-thiophosphoric triamide, a suicide substrate: structure and kinetics"

Biochemistry **2017**, *56*, 5391-5404

IF: 2.997

#144 V. Broll; A. H. S. Martinelli; F. C. Lopes; L. L. Fruttero; B. Zambelli; E. Salladini; O. Dobrovolska; S. Ciurli*; C. Carlini*

"Structural analysis of the interaction between Jaburetox, an intrinsically disordered protein, and membrane models"

Colloids Surf. B, **2017**, *159*, 849-860

IF: 3.997

#143 M. Palombo; A. Bonucci; E. Etienne; S. Ciurli; V. N. Uversky; B. Guigliarelli; V. Belle; E. Mileo*; B. Zambelli*

"The relationship between folding and activity in UreG, an intrinsically disordered enzyme"

Sci. Rep. **2017**, *7*, 5977

IF: 4.122

#142 M. Masetti*; F. Musiani*; M. Bernetti; F. Falchi; A. Cavalli; S. Ciurli; M. Recanatini

"Development of a multisite model for Ni(II) ion in solution from thermodynamic and kinetic data"

J. Comp. Chem. **2017**, *38*, 1834-1843

IF: 3.221

#141 J. Timm; C. Brochier-Armanet; J. Pérard; B. Zambelli; S. Ollagnier-de-Choudens; S. Ciurli; C. Cavazza*
 "The CO dehydrogenase accessory protein CooT is a novel nickel-binding protein"
Metalomics **2017**, *9*, 575-583
 IF: 4.069

#140 C. Carr; F. Musiani; H.-T. Huang; P. T. Chivers; S. Ciurli; M. J. Maroney*
 "Glutamate ligation in the Ni(II) and Co(II) responsive *E. coli* transcriptional regulator, RcnR"
Inorg. Chem. **2017**, *56*, 6459-6476
 IF: 4.700

#139 F. Musiani; D. Gioia; M. Masetti; F. Falchi; A. Cavalli; M. Recanatini; S. Ciurli*
 "Protein tunnels: the case of urease accessory proteins"
J. Chem. Theory Comp. **2017**, *13*, 2322-2331
 IF: 5.399

#138 L. Mazzei; F. Musiani; S. Ciurli*
 "Urease"
RSC Metallobiology - Book Series "The Biological Chemistry of Nickel", **2017**, pp. 60-97.

#137 L. Mazzei; M. Cianci; F. Musiani; G. Lente; M. Palombo; S. Ciurli*
 "Inactivation of urease by catechol: kinetics and structure"
J. Inorg. Biochem., **2017**, *166*, 182-189
 IF: 3.063

#136 E. Fabini; B. Zambelli; L. Mazzei; S. Ciurli*; C. Bertucci*
 "Surface plasmon resonance and isothermal titration calorimetry to monitor the Ni(II)-dependent binding of *Helicobacter pylori* NikR to DNA"
Anal. Bioanal. Chem. **2016**, *408*, 7971-7980

#135 R. Borghese*; L. Canducci; F. Musiani; M. Cappelletti; S. Ciurli; R. Turner; D. Zannoni
 "On the role of a specific insert in acetate permeases (ActP) for tellurite uptake in bacteria: functional and structural studies"
J. Inorg. Biochem. **2016**, *163*, 103-109
 IF: 3.307

#134 B. Zambelli; V. Uversky; S. Ciurli*
 "Nickel impact on human health: an intrinsic disorder perspective"
BBA Proteins Proteom. **2016**, *1864*, 1714-1731
 IF: 2.773

#133 L. Mazzei; M. Cianci; F. Musiani; S. Ciurli*
 "Inactivation of urease by 1,4-benzoquinone: chemistry at the protein surface"
Dalton Trans. **2016**, *45*, 5455-5459
 IF: 4.029

#132 L. Mazzei; M. Cianci; S. Benini; L. Bertini; F. Musiani; S. Ciurli*
 "Kinetic and structural studies reveal a unique binding mode of sulfite to the nickel center in urease"
J. Inorg. Biochem. **2016**, *154*, 42-49
 IF: 3.338

#131 L. Mazzei; S. Ciurli*; B. Zambelli
 "Isothermal titration calorimetry to characterize enzymatic reactions"
Methods Enzymol. **2016**, *567*, 215-234
 IF: 1.972

#130 L. Mazzei; O. Dobrovolska; F. Musiani; B. Zambelli; S. Ciurli*
 "On the interaction of *Helicobacter pylori* NikR, a Ni(II)-responsive transcription factor, with the urease operator: in solution and in silico studies"
J. Biol. Inorg. Chem. **2015**, *20*, 1021-1037
 IF = 2.495

#129 F. Musiani*; S. Ciurli*
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