



**FIRST CONFERENCE
OF THE ITALIAN
BIOINORGANIC
CHEMISTRY GROUP**

FULL PROGRAMME

SEPTEMBER 7-9, 2026

COMPLESSO DEI SS. MARCELLINO E FESTO

Conference Center of the University of Naples Federico II

NAPLES, ITALY



**Società
Chimica
Italiana**

Gruppo Tematico di
Chimica Bioinorganica

www.itabic26.unina.it



Welcome to the First Italian Bioinorganic Chemistry Conference ItaBIC26!

The Scientific and Organizing Committees are delighted to welcome you to the inaugural conference of the **Bioinorganic Chemistry Group** of the **Società Chimica Italiana (SCI)**, hosted by the University of Naples Federico II, in the historic setting of Naples, Italy. ItaBIC26 aims to bring together the Italian and international bioinorganic chemistry communities to discuss recent advances at the interface between **Inorganic Chemistry** and the **Life Sciences**, promoting scientific exchange, networking and new collaborations.

The scientific program features **three Plenary Lectures** delivered by internationally renowned scientists, **Thomas R. Ward** (University of Basel, Switzerland), **Franc Meyer** (Georg-August-Universität Göttingen, Germany), and **Gilles Gasser** (Chimie ParisTech, PSL University, France), together with **five Keynote Lectures** presented by distinguished experts: **Anabella Ivancich** (CNRS and Aix-Marseille University, France), **Fabio Carniato** (Università del Piemonte Orientale, Italy), **Gianantonio Battistuzzi** (Università di Modena e Reggio Emilia, Italy), **Ulf Hanefeld** (Delft University of Technology, The Netherlands), and **Emilia Sicilia** (Università della Calabria, Italy). The program is further enriched by **40 oral communications** and **more than 30 poster presentations**, offering a broad overview of the current and vibrant research activities in the field.

These three days will represent a valuable opportunity for scientific discussions and interactions among researchers working on the many aspects of **bioinorganic chemistry**, including metal ions in biology and medicine, metalloproteins and metalloenzymes, metal-based therapeutics, bioinspired catalysis, spectroscopy, computational approaches, and chemical biology.

The Organizing Committee gratefully acknowledges all invited speakers, participants, sponsors, and supporting organizations for their contribution to the success of this first edition. We look forward to welcoming you to Naples and to an inspiring meeting full of scientific exchange and collaboration.

The Scientific and Organizing Committees

SCIENTIFIC COMMITTEE

Francesco Paolo Fanizzi

Università del Salento

Angelina Lombardi

Università degli Studi di Napoli Federico II

Tiziana Marino

Università della Calabria

Riccardo Pettinari

Università degli Studi di Camerino

Alessandro Pratesi

Università di Pisa

Michele Saviano

Consiglio Nazionale delle Ricerche



ORGANIZING COMMITTEE

Angelina Lombardi (co-chair)

Flavia Nastri (co-chair)

Stefania Galdiero (co-chair)

Marco Chino

Daniele D'Alonzo

Maria De Fenza

Alessandra Esposito

Linda Leone

Domenico Loreto

Ornella Maglio

Rosa Bellavita

Sara La Manna

Daniela Marasco



UNIVERSITÀ DEGLI STUDI DI NAPOLI
FEDERICO II



We gratefully acknowledge our partners and sponsors:



HORIBA

deltek D>

OPST
OLIGO PEPTIDE SERVICE TECHNOLOGY

VACUUM SERVICE
Vacuum Technologies & Service



OCF ORDINE REGIONALE
DEI CHIMICI E DEI FISICI
DELLA CAMPANIA



neapōlis
UNIVERSITÀ DEGLI STUDI DI NAPOLI FEDERICO II
SCUOLA POLITECNICA E DELLE SCIENZE DI BASE

CON IL PATROCINIO DEL
COMUNE DI NAPOLI



CONFERENCE GUIDE

SCIENTIFIC INFORMATION

ORAL PRESENTATIONS

It is of the utmost importance that you respect the allocated time to avoid any delay of the sessions during the conference.

A laptop PC will be available in the conference room. Speakers are kindly requested to upload their presentation in PPT or PDF file format the day before or during the break preceding their allocated session at the latest.

Presentation Formats

Code	Presentation Type	TIME	Q&A	Total
PL	Plenary Lecture	40 min	5 min	45 min
KL	Keynote Lecture	25 min	5 min	30 min
GOC	Gold Oral Communication	17 min	3 min	20 min
*OC	Oral Communication	13 min	2 min	15 min
OC	Oral Communication	8 min	2 min	10 min

The official language of the conference will be English

POSTER PRESENTATIONS

Posters can be fixed on the dedicated boards located in the room adjacent to the Main Hall on September 7 in the morning and removed on September 9 at the end of the Meeting. Boards will be numbered as per the scientific program, so Presenters are kindly requested to fix their poster on the corresponding board.

Pins are provided by the organizing secretariat



GENERAL INFORMATION

VENUE

Located in the Historic City Centre of Naples, the Conference Center of the University of Naples Federico II is housed in the **Complesso dei Santi Marcellino e Fesito**, a prestigious venue that blends cultural heritage with modern facilities.

REGISTRATION DESK & CONFERENCE SECRETARIAT

The Registration Desk will be located at the entrance of the conference venue and will remain open throughout the meeting. Participants can collect their conference materials and badges upon arrival, and the staff will be available to provide assistance and information regarding the scientific programme, social events and general conference logistics.

For any questions during the conference, please contact the
Conference Secretariat at ambralab@unina.it

Throughout the conference, members of the Organizing Committee will be available to assist participants.

COFFEE BREAKS AND LUNCHES

Coffee breaks and lunches are included in the registration fee and will be served according to the scientific programme.

GALA DINNER

The Gala dinner is organized on September 8th at h. 20.30 for all registered participants. It will be held at the exclusive **Reale Yacht Club Canottieri Savoia** located in Banchina S. Lucia, 13, 80132 Napoli. The Club is located in front of from Castel dell'Ovo.

Gentlemen are kindly requested to wear a jacket and tie

AWARDS

The Organizing Committee is delighted to announce that Frontiers (Frontiers | Publisher of peer-reviewed articles in open access journals) will support four awards dedicated to the best scientific contributions presented at the congress. The **two Best Poster Presentation Awards** and the **two Best Oral Presentation Awards** will be assigned to recognize excellence in scientific content, originality, presentation quality and communication effectiveness. Each award will consist of a monetary prize, generously sponsored by **Frontiers**. Awardees will be selected by the Scientific Committee and announced during the final session of the congress. In addition, Frontiers will identify one selected contributor who will be offered the opportunity to submit a manuscript to **Frontiers in Drug Discovery** with publication fees waived. The manuscript will be subject to the journal's standard editorial and peer-review process.

ATTENDANCE CERTIFICATE

An attendance certificate and the payment receipt will be sent by email to all registered participants at the end of the conference.

WIFI ACCESS

Complimentary Wi-Fi will be available throughout the conference venue.

- Network (SSID): ITABIC26
- Password: Conference@26

PHOTOGRAPHY

Please note that photographs and videos may be taken during the conference for promotional/social purposes. By attending the conference, participants consent to the use of these images unless otherwise requested.

SOCIAL MEDIA

Participants are encouraged to share their conference experience using the official hashtag: **#ITABIC26**

Monday, **September 7th, 2026**

12:00	Registration
14:00 – 14:30	Welcome and Opening Ceremony
SESSION 1 Mechanistic Insight in Binding and Activity Chairs: Michele Saviano and Marco Chino	
14:30 – 15:00	[KL01] • Gianantonio Battistuzzi Dipartimento di Scienze Chimiche e Geologiche Università di Modena e Reggio Emilia, Italy Reduction thermodynamics to unravel the molecular factors influencing the E° of redox metalloproteins
15:00 – 15:15	[*OC01] • Miriam Malagnini Aix-Marseille University Marseille, France Electrochemical characterization of <i>C. pasteurianum</i> hydrogenase II and four site-directed variants: catalysis and inhibition
15:15 – 15:30	[*OC02] • Mario Prejanò Università della Calabria Effect of distal aminoacidic mutations to Fe(III)/Fe(II) redox potential in human neuroglobin: insights from molecular modeling
15:30 – 15:40	[OC01] • Mirco Meglioli Università di Modena e Reggio Emilia Role of Distal Residues in Controlling the Interaction of Hydrogen Sulfide with Neuroglobin
15:40 – 15:55	[*OC03] • Chiara Bacchella Università degli Studi di Pavia The Many Faces of Metal Ions in Neurodegeneration
15:55 – 16:10	[*OC04] • Luigi Russo Università degli Studi della Campania "Luigi Vanvitelli" Mechanistic Insights into the Early Events of Prion Protein Pathogenic Conversion
16:10 – 16:40	Coffee Break

SESSION 2a

Natural and Artificial Metalloenzymes

Chairs: Angela Lombardi and Matteo Tegoni

16:40 – 17:25	[PL01] • Thomas R. Ward University of Basel and National Center of Competence in Research "Molecular Systems Engineering", Switzerland Artificial and Repurposed Metalloenzymes for in vivo New-to-Nature Catalysis Challenges and Opportunities
17:25 – 17:45	[GOC01] • Francesca Valetti Università di Torino Deciphering H-Cluster Protection Mechanisms in [FeFe]-Hydrogenases for the Design of Oxygen-Tolerant Catalysts
17:45 – 18:00	[*OC05] • Lorena Simunic Università degli Studi di Napoli Federico II Artificial metalloenzymes inspired by LPMOs for waste valorization
18:00 – 18:10	[OC02] • Roberta Russo Università degli Studi di Napoli Federico II Exploring the catalytic potential of a miniaturized heme enzyme in new-to-nature reactions
18:10 – 18:40	[KL02] • Ulf Hanefeld Biokatalyse, Afdeling Biotechnologie, Technische Universiteit Delft, HZ Delft, The Netherlands Versatility and Surprises with Manganese in Biocatalysis
19:00 – 21:00	Welcome Light Aperitif

Tuesday, **September 8th, 2026**



SESSION 2b Natural and Artificial Metalloenzymes Chairs: Flavia Nastri and Maria Elisa Crestoni	
9:30 – 10:00	[KL03] • Anabella Ivancich French National Centre for Scientific Research (CNRS) and Aix-Marseille University Marseille, France De novo designed alpha-helical heme proteins as structural/functional models of bi-functional KatGs and cyt P450 peroxxygenases
10:00 – 10:15	[*OC06] • Federica Arrigoni Università degli Studi di Milano-Bicocca Multiscale Computational Insights into the Structure-Function Relationships of [FeFe]-Hydrogenases
10:15 – 10:25	[OC03] • Iago De Assis Modenez French National Centre for Scientific Research (CNRS) and Aix-Marseille University Marseille Probing Nε- and Nδ-histidine ligation in a de novo designed α-helical heme protein
10:25 – 10:35	[OC04] • Chiara Elena Palmiero Università degli Studi di Napoli Federico II MetalHawk 2.0: Beyond Octahedral Geometries with Neural Network Classification of Metal Sites
10:35 – 10:45	[OC05] • Alessia Procentese Università degli Studi di Napoli Federico II Design, synthesis, and characterization of a stimuli-responsive peptide-based hydrogel
10:45 – 10:55	[OC06] • Oluwasegun Eric Ajayi Università degli Studi di Siena Copper calling: Myxinidin and the ATCUN motif in metal binding
10:55 – 11:30	Coffee break and Poster Session

SESSION 3

Biocatalysis: Theoretical and Experimental Approaches

Chairs: Tiziana Marino and Roberto Fattorusso

11:30 – 11:50	[GOC02] • Luca Bertini Università degli Studi di Milano-Bicocca How Do Laccases Oxidize Recalcitrant Substrates? Insights from Classical and DFT Modeling
11:50 – 12:05	[*OC07] • Rachele Zunino Università degli Studi di Napoli Federico II QM/MM Investigation of O₂ Binding at the Binuclear Copper Active Site of Arthropod Hemocyanins: Insights Across Arthropod Lineages
12:05 – 12:20	[*OC08] • Rajesh Kushwaha University of Strasbourg Biologically Robust Copper(I) Photocatalysis Enables Oxidation of Endogenous Reductants under Aqueous Conditions
12:20 – 12:30	[OC07] • Jishnu Sai Gopinath Czech Academy of Sciences A Simple yet Efficient Model for Computing H-Atom Transfer Tunneling from Transition-State Properties
12:30 – 13:15	[PL02] • Franc Meyer Institut für Anorganische Chemie, Georg-August-Universität Göttingen, Germany Bioinspired Dicopper/Dioxygen Chemistry: New Intermediates, Electronic Structures, and Reactivities
13:15 – 14:30	Light Lunch and Poster Session

SESSION 4a

Metals in Medicine and Diagnostics

Chairs: Stefania Galdiero and Alessandro Pratesi

Saluti istituzionali di **Rossella Fasulo**,

Presidente Ordine Regionale dei Chimici e dei Fisici della Campania

14:30 – 15:00	[KL04] • Fabio Carniato Dipartimento di Scienze ed Innovazione Tecnologica Università degli Studi del Piemonte Orientale, Italy Novel Mn(II)- and Fe(III)-based probes as alternatives to conventional Gd(III) MRI contrast agents
----------------------	--

15:00 – 15:20	[GOC03] • Luigi Messori Università degli Studi di Firenze Metal compounds as prospective antibacterial agents. Case Studies
15:20 – 15:35	[*OC09] • Thomas Scattolin Università degli Studi di Padova Gold(I)–NHC Complexes Bearing Non-Steroidal Anti-Inflammatory Drugs: An Innovative Synthetic Approach and Antitumor Activity
15:35 – 15:50	[*OC10] • Diego Di Girolamo Università degli Studi di Roma Tor Vergata NAM-Oriented In Silico Dermatokinetic Modeling of TiO₂ and Cu-Phthalocyanine Tattoo Pigments for Risk Assessment
15:50 – 16:00	[OC08] • Simone Braccia Università degli Studi di Napoli Federico II Fe(III) coordination and membrane interaction drive the enhanced antimicrobial activity of a siderophore-peptide conjugate
16:00 – 16:30	Coffee Break and Poster Session
SESSION 4b Metals in Medicine and Diagnostics Chairs: Maria Pia Donzello and Riccardo Pettinari	
16:30 – 16:45	[*OC11] • Diego Tesauo Università degli Studi di Napoli Federico II Insights into on the behaviour of N-Heterocyclic Carbene (NHC) Gold(I) complexes targeting the Thioredoxin System
16:45 – 17:00	[*OC12] • Lara Massai Università degli Studi di Firenze Metal-Based Anticancer Drugs Targeting Cytochrome c: Molecular Insights and Clinical Perspectives
17:00 – 17:15	[*OC13] • Erika Ferrari Università di Modena e Reggio Emilia Charge Matters: A Sulfonated TACN Chelator Enabling Neutral and Stable Cu(II) Complexes for ⁶⁴Cu radiopharmaceuticals

17:15 – 17:30	[*OC14] • Gina Elena Giacomazzo Università degli Studi di Firenze From Metal Complexes to Clinical Application: Ru(II)- and Os(II)-based Photosensitizers for PDT of Vulvar Intraepithelial Neoplasia
17:30 – 17:40	[OC09] • Erika Stefàno Università del Salento NMR-Based Metabolomic Approach revealed different response of Pancreatic Ductal Adenocarcinoma cells to [Pt(O,O'-acac)(γ-acac)(DMS)] and cisplatin treatment
17:40 – 17:50	[OC10] • Lorenzo Risolo Università del Piemonte Orientale Fluoride Coordination in Metal Complexes: Thermodynamic, Kinetic and Structural Insights for Sensing and Diagnostic Applications
17:50 – 18:00	[OC11] • Giulia Marcolli Politecnico di Milano Enhanced metal ion recognition with bispidine-based fluorinated chemosensors
20:30	Social Dinner

Wednesday, **September 9th, 2026**

SESSION 5 Metal-based drugs: Theoretical and Experimental Approaches Chairs: Michele Benedetti and Giorgio Pelosi	
9:30 – 10:00	[KL05] • Emilia Sicilia Dipartimento di Chimica e Tecnologie Chimiche, Università della Calabria, Arcavacata di Rende, Italy Computational insights on the anticancer activity of redox-activated Pt(IV) complexes
10:00 – 10:15	[*OC15] • Tiziano Marzo Università di Pisa Human Serum Albumin: A Hidden Player in the Success of Anticancer Metallodrugs
10:15 – 10:30	[*OC16] • Mauro Ravera Università del Piemonte Orientale An Unsymmetric Cisplatin-Based Pt(IV) Compound Containing 2-(2-Propynyl)Octanoate: A Coin With Many Faces
10:30 – 10:40	[OC12] • Giovanni Tonon Università di Venezia Harnessing Mesoionic Carbenes: Synthesis and Antiproliferative Activity of Novel Steroidal Metal Bioconjugates
10:40 – 10:50	[OC13] • Daniele Belletto Università della Calabria Passive diffusion of cisplatin and cisplatin-derived Pt(IV) prodrugs across a breast cancer plasma membrane: computational insights into the role of axial ligands
10:50 – 11:00	[OC14] • Alessia Dodaro Università della Calabria Advanced computational investigation of human Transferrin as a vehicle for metallodrugs absorption against cancer
11:00 – 11:30	Coffee break

SESSION 6

Metals in Medicine

Chairs: Daniela Marasco and Francesco Paolo Fanizzi

11:30 – 12:15	[PL03] • Gilles Gasser Chimie ParisTech, PSL University, CNRS Institute of Chemistry for Life and Health Sciences (i-CLeHS), France Metal Complexes for Medicinal Applications
12:15 – 12:25	[OC15] • Federica De Castro Università del Salento Sub-Lethal Stress vs Cytotoxic Threshold: Metabolic Rewiring of Neuroblastoma Cells Exposed to [Pt(η^1-C₂H₄OMe)(DMSO)(phen)]⁺ complex
12:25 – 12:35	[OC16] • Anna Maria Di Cosola Università degli Studi di Bari In vitro and ex vivo evaluation of dinuclear platinum–bisphosphonate complexes against prostate cancer bone metastasis models
12:35 – 12:45	[OC17] • Lorenzo Luciani Università di Camerino Carbazole-Based NHC Cu(I) And Au(I) Complexes As Anticancer Agents
12:45 – 12:55	[OC18] • Claudia Ghelarducci Università di Pisa Novel Pt(II) Complex-Peptide Conjugates for Targeted Anticancer Therapies: Synthesis, Characterization, and Bioactivity
12:55 – 13:10	[*OC17] • Damiano Cirri Università di Pisa Iodide in Gold and Platinum Anticancer Complexes: Reactivity Is Not Activity
13:10 – 13:30	[GOC04] • Annie Castonguay INRS, Institut national de la recherche scientifique, Canada Design of biologically active ruthenium-based organometallic complexes
13:30	Awards and Concluding Remarks

List of Posters

PO01	Anna Giorgio	Università degli Studi di Napoli, CNR, IBB
	Development of novel $[^{99m}\text{Tc}][\text{Tc}(\text{N})(\text{PNP})]$ -labeled peptides for the diagnosis of $\alpha\text{V}\beta 3$ -positive cancers	
PO02	Mattia Fanelli	Università degli Studi di Firenze
	Deciphering the Mode of Action of Anticancer Gold Compounds via Shotgun Proteomics and Bioinformatics	
PO03	Erika Stefàno	Università del Salento
	Study of $[\text{Pt}(\text{O}, \text{O}'\text{-acac})(\gamma\text{-acac})(\text{DMS})]$ and cisplatin anticancer activity on Pancreatic Ductal Adenocarcinoma cells	
PO04	Rossana Galassi	Università di Camerino
	New Details on the Anticancer Activity of Imidazolyl based Gold(I) Complexes	
PO05	Martina Aguanno	Università degli Studi di Firenze
	Advanced LC-MS strategies for the characterization of metal/protein adducts: methodological optimization and oncological applications	
PO06	Lorenzo Emiliano Imbò	Università degli Studi di Napoli Federico II
	Exploring Fe(III) coordination and membrane interaction of a siderophore-peptide conjugate: Enhancing synergistically the antimicrobial activity	
PO07	Francesca Fasano	Scuola Superiore Meridionale
	ATCUN-Mediated Copper Binding in Myxinidin	
PO08	Chiara Gabbiani	Università di Pisa
	Highly Cytotoxic Gold(I) Complexes Bearing Anthracenyl-Functionalized Phosphine Ligands	
PO09	Attilio Squadrini	Università di Parma
	Design and Antitumoral Evaluation of a Bioconjugable Copper(II)-Thiosemicarbazone Complex: ROS Targeting and Cytotoxicity in HT29 and A549 Cell Lines	
PO10	Dominga Rogolino	Università di Parma
	Thiohydrazones and their copper(ii) complexes as bioactive compounds	
PO11	Susanna Grasso	Sapienza Università di Roma
	Auranofin binding to uracil and thiouracils assayed by IRMPD spectroscopy	

PO12	Miriam Caviglia	Università di Camerino
	Copper and silver complexes as next-generation metallodrugs for the treatment of resistant cancers	
PO13	Valentina Ceccherini	Università degli Studi di Firenze
	Metal-Based Complexes as Emerging Antibacterial Agents: An Overview of Novel Design Strategies	
PO14	Andrea Angelucci	Sapienza Università di Roma
	Synthesis, physico-chemical properties and In Vitro studies of new porphyrazine complexes of the lanthanide series. Exploration of their potential applications in biomedicine	
PO15	Valentina Pecchioli	Università degli Studi di Firenze
	Exploring ferroptosis-related metabolomic signature of gold-based anticancer compounds: comparison with Erastin in A2780 ovarian cancer cells	
PO16	Vinay Kumar Srivastava	D.S College, Aligarh, India
	MoS ₂ Nanoparticles Derived from a Bioactive Pyrrolidine Dithiocarbamate Molybdenum(V) Complex	
PO17	Diego Di Girolamo	Università di Roma Tor Vergata
	The impact of cavitation treatments on optical properties, aggregation and toxicity of PG7 and PY14	
PO18	Jitka Pracharova	Palacký University Olomouc
	Antimetastatic Activity of a Novel (Arene)Ruthenium(II) Naphthopyran Complex in Metastatic Cancer Models	
PO19	Nicola Garofalo	Università del Salento
	Synthesis of Platinum(II) complexes with chelating amines: a greener approach using water/choline chloride-based deep eutectic solvents	
PO20	Chiara Santoni	Università Politecnica delle Marche
	Reducing chemoresistance in Triple-Negative Breast Cancer through PON2 silencing: FTIRM insights into response to combined therapy	
PO21	Martyna Kapica	University of Gdańsk, Poland
	Electrostatically-driven assembly of cationic lipopeptides with hexacyanoferrate anions: a thermodynamic and in silico study	
PO22	Matteo Tegoni	Università di Parma
	(The Power of) Vision3D: creating new virtual environments for 3D protein visualization and science dissemination	
PO23	Matteo Tegoni	Università di Parma
	Evolving SpyTag/SpyCatcher system into new artificial proteins	

PO24	Francesco Giaretto	Università di Torino
	Structural characterization of the chimeric enzyme CYP-SOX by pulsed EPR spectroscopy	
PO25	Hansol Kim	SoonChunHyang University
	Single-site hydrogen-bond modulation enhances catalytic ester hydrolysis in a Zn(II)-TPA scaffold	
PO26	Alessandra Esposito	Università degli Studi di Napoli Federico II
	Coupling Artificial Metalloenzymes with Photosensitizers for H ₂ Evolution	
PO27	Maria De Fenza	Università degli Studi di Napoli Federico II
	From nitrogen to sulfur ligation: reprogramming reactivity in miniaturized heme enzymes	
PO28	Luisa Curlacci	Università degli Studi di Bari
	Metal Binding Dynamics in Human Ctr1(1–25): A pH-Dependent Coordination Switch	
PO29	Domenico Loreto	Università degli Studi di Napoli Federico II
	Design, Synthesis and Characterization of a Zn(II)His ₃ Site in a Heterodimeric Three-Helix Bundle Scaffold	
PO30	Simone Molinaro	Università degli Studi di Napoli Federico II
	Artificial Type II copper proteins: a spectroscopic characterization	
PO31	Naveen Kumar	Università degli Studi di Napoli Federico II
	Oxidative biotransformation of lignin by a miniaturized heme-enzyme	
PO32	Concetta Avitabile	Istituto di Cristallografia- CNR
	Ruthenium Hexamine-Mediated Paper-Based PNA Biosensor for Pancreatic Ductal Adenocarcinoma Diagnosis	

Bioinorganic Chemistry in Medicine and Nanotechnology
Spectroscopic and computational methods
Natural and artificial metalloenzymes
Bioinorganic compounds in sensing and diagnostics

