



eBIC 2021 *Program*

July 20–22, 2021, 8 am GMT

Plenary lectures: 45 minutes

Invited lectures: 20 minutes

Video flash presentations: 4 minutes pre-recorded, live questions

July 20, 2021

Session Chairs: *Paul Walton and Nick LeBrun*

GMT	Local Time	Speaker	Title
8:00	10 am (Paris)	Vincent L. Pecoraro	<i>Welcome to eBIC</i>
8:05	10:05	Isabelle Schalk	<i>How P. aeruginosa accesses iron according to its environment: molecular mechanisms and phenotypic adaptation</i>
9:00	11:00	Takahiko Kojima	<i>Mechanistic insights into C-H oxidation by Ru(IV)-oxo complexes</i>
9:30	11:30	Sonia Infante-Tadeo	<i>Osmium(II) Tethered Half-Sandwich Complexes</i>
		Slawomir Potocki	<i>Characterization of Zinc Complexes with $\alpha 5$ Domains of Mycobacterial ArsR Family Proteins</i>
		Monica Cziferszky	<i>Using MS to get insights into the molecular interactions of metal complexes with biomolecules</i>
		Claudia Schmidt	<i>Cyclometalated Gold Complexes for the Identification of Target Proteins in Bacteria</i>
		Efrosini Kioseoglou	<i>Advanced Vanadium Peroxido Materials in Biological Systems</i>
		Veronica Ghini	<i>NMR Reveals the Metabolic Changes Induced by Auranofin in Ovarian Cancer Cells</i>
10:30	12:30	Lizhu Wu	<i>Artificial Photosynthesis for Chemical Transformation</i>
11:00	13:00	Jalila Simaan	<i>Copper-containing Lytic Polysaccharide Monooxygenases: Biological system and bioinspired models</i>
11:30	13:30	Dinorah Gambino	<i>Designing multifunctional prospective antiparasitic metal-based compounds</i>
12:00	14:00	BREAK	

July 20, 2021

Session Chairs: *Clotilde Policar and Anabella Ivancich*

GMT	Local Time	Speaker	Title
12:30	14:30 (Paris)	Sigríður Suman	<i>Biological Studies of Molybdenum Sulfur Complexes and Influence on Cyanide Inhibition of Cytochrome c Oxidase</i>
13:00	15:00	Joanna Lachowicz	<i>Thymosin b4 is an endogenous iron chelator and molecular switcher of ferroptosis</i>
13:30	15:30	Mauro Ravera	<i>A Proof of Concept Study for Increasing the antiproliferative activity of Pt(IV) Bifunctional Prodrugs with Hadrons</i>
		Anton Kovalenko	<i>Polystyrene Nanoparticles Doped with Lanthanide Complexes for Photoacoustic and Near-Infrared Luminescence Imaging</i>
		Darren Griffith	<i>Tumour Targeting of an Oxaliplatin-based Chemotherapeutic Regimen Using Ultrasound Targeted Microbubble Destruction</i>
14:00	16:00	Anthony Green	<i>Tuning Metal-Oxo Reactivity in Enzyme Active Sites using an Expanded Genetic Code</i>
14:30	16:30	Sarah Michel	<i>Iron sulfur clusters masquerading as zinc finger proteins</i>
15:00	17:00	Jennifer Bridwell-Rabb	<i>Metalloprotein Design Principles for Site-Selective Hydroxylation</i>
15:30	17:30	BREAK	

July 20, 2021

Session Chairs: Vincent L. Pecoraro and Kathy Franz

GMT	Local Time	Speaker	Title
16:00	12:00 (NY)	Vincent L. Pecoraro	<i>Welcome to eBIC</i>
16:05	12:05	David Giedroc	<i>Metals, molecules and metabolism: Molecular mechanisms of bacterial metallostasis</i>
17:00	13:00	Carole Duboc	<i>From H₂ production to CO₂ reduction with the same bio-inspired NiFe complex</i>
17:30	13:30	Luiz Antônio Costa	<i>A Molecular Dynamics Study of Non-Covalent Interactions Between SI-PPCS and Biomolecules</i>
		Magali Scocozza	<i>Spectroelectrochemical Characterization of a Type-A Dye Decoloring Peroxidase</i>
		Jing Yang	<i>Mo K-edge XAS and Bond Valence Sum Analysis</i>
		Ferianys Rivas	<i>Heterobimetallic ferrocenyl antiparasitic compounds: a QSAR study</i>
		Teresa Nava-Ramirez	<i>Chaperone activity of the C-terminal domain of large-size subunit catalases: molecular mechanism</i>
		Carlos Yañez	<i>Development of Cu(II)-L-dipeptide-3,4,7,8- tetramethyl phenanthroline complexes in the search of new drugs to treat cancer</i>
		John Vincent	<i>A role for LMWCr in Transferrin-mediated Cr(III) Transport</i>
18:30	14:30	Thorifinnur Gunnlauggsson	<i>Ru(II) polypyridyl complexes as DNA binders, cellular imaging and light activated therapeutic agents</i>
19:00	15:00	Arthur Tinoco	<i>A closed protein conformation is not a requirement for metal cellular uptake via transferrin endocytosis</i>
19:30	15:30	Maria Contel	<i>Antibodies as targeting vectors for HER-2 positive breast cancer gold-based chemotherapeutics</i>
20:00	16:00	BREAK	

July 20, 2021Session Chairs: *Andy Borovik and Michael Green*

GMT	Local Time	Speaker	Title
20:30	16:30 (NY)	Sherri McFarland	<i>Metallo drug Design for Light-Based Cancer Therapy</i>
21:00	17:00	Tim Storr (ECR2021)	<i>Designing Multifunctional Molecules to Control Protein Misfolding</i>
22:00	18:00	Alexander Spokoyny	<i>Organometallic Reagents for Bioconjugation</i>
22:30	18:30	David Wright	<i>Inorganic applications for signal amplification in low resource diagnostics</i>
23:00	19:00	Elizabeth New	<i>Fluorescent sensors to study the biological interactions of platinum-based chemotherapeutic agents</i>
23:30	19:30	BREAK	

July 21, 2021

Session Chairs: *Christian Hartinger and Guy Jameson*

GMT	Local Time	Speaker	Title
00:00	8:00 (Beijing)	Vincent L. Pecoraro	General Assembly
01:00	9:00	Stephen Bell	<i>To be, or not to be an inhibitor; a comparison of inhibitor/substrate interactions with ferric and ferrous heme in cytochrome P450 enzymes</i>
01:30	9:30	Saawan Kumar	<i>Tumour Targeting Peptides in Cancer Therapy</i>
		Matthew Sullivan	<i>Delving into the Exquisite Specificity of Plecstatin-1</i>
		Jiarun Lin	<i>Novel multimodal probes for cellular imaging</i>
02:00	10:00	Vivian Yam	<i>From Discrete Metal Complexes to Ensembles and Assemblies for Sensing, Molecular Imaging and Bioassays</i>
03:00	11:00	Shinobu Itoh	<i>Copper Action in Type-3 Copper Monooxygenase</i>
03:30	11:30	Junlong Zhang	<i>Lanthanide Porphyrinoid Molecular Phototheranostics</i>
04:00	12:00	BREAK	

July 21, 2021

Session Chairs: *Hongzhe Sun and Guangyu Zhu*

GMT	Local Time	Speaker	Title
04:30	12:30 (Beijing)	Jaehung Cho	<i>Small molecule activation for enzyme inhibition and cell signaling</i>
05:00	13:00	Ankona Datta	<i>Sensors for Tracking Mn²⁺ ions in Living Cells: Why? How? and Where?</i>
05:30	13:30	Lewis Green	<i>Immunogenic Cell Death: Reawakening the Immune system to</i>
		TaoTao Zou	<i>Cancerous Threats with Chemotherapeutic Compounds</i>
		Ashley Hollings	<i>Gold Based Anti-Cancer Prodrugs With Stimuli Activatable Properties</i>
			<i>XANES Studies of Brain Zinc Homeostasis and its Role During Cognitive Decline and Ageing</i>
6:00	14:00	Arindam Mukherjee	<i>Cytotoxic activity of Mesalazine based Ru(II) complexes against NOTCH1 active oral cancer stem cells (CSCs): Inducing differentiation and killing CSCs</i>
6:30	14:30	Ulrich Schatzschneider	<i>Novel bioconjugation methods for metal complex functionalization of peptides and proteins</i>
7:00	15:00	Ricardo Louro	<i>Extracellular electron transfer in Gram-positive and Gram-negative bacteria: the same, but different</i>
07:30	15:30	BREAK	

July 21, 2021

Session Chairs: *Celine Marmion and Stéphane Petoud*

GMT	Local Time	Speaker	Title
8:00	10 am (Paris)	Erwin Reisner	<i>The Role of Bioinorganic Chemistry in Artificial Photosynthesis</i>
9:00	11:00	Chunying Chen	<i>Roles of the Protein Corona in Nanomedicine: from analytical approaches to applications</i>
9:30	11:30	Anna Peacock	<i>Coiled coils as ligands for inclusion in the inorganic chemist's toolbox</i>
10:00	12:00	BREAK	
10:30	12:30	Nora Kulak Silvia Ciambellotti Sevasti Matsia	<i>ATCUN Metallopeptides: Towards Efficient DNA Cleavage Agents</i> <i>Photosensitizing Ferritin-Based Nanocomposites Bearing Ru(II) Complexes</i> <i>Structure-Bioactivity Correlations in Binary Thallium Hydroxycarboxylic Acid Systems</i>
11:00	13:00	Norbert Bedő Lena Daumann	<i>Interaction of Cytochrome c Oxidase with Molybdenum Complexes</i> <i>The role of lanthanides and actinides in alcohol oxidation: enzymes and biomimetics</i>
11:30	13:30	Lucia Banci	<i>Molecular description of FeS proteins biogenesis</i>
12:00	14:00	BREAK	

July 21, 2021

Session Chairs: *Elzbieta Gumienna-Kontecka and Alicia Dominguez-Martin*

GMT	Local Time	Speaker	Title
12:30	14:30 (Paris)	Takashi Hayashi	<i>Engineering of Hemoproteins to Create Artificial Metalloenzymes</i>
13:00	15:00	Alejandro Vila	<i>Periplasmic hideouts of metallo-beta-lactamases to escape zinc starvation</i>
13:30	15:30	Kamila Stokwoa-Sołtys	<i>F.nucleatum Outer Membrane Proteins Increase Prooxidant Activity of Cu(II) Ions</i>
		Thiago Valdares de Oliveira	<i>Cyanide as a Public Health Issue: Mechanistic Approach with water soluble α-amino acid complexes with Molybdenum</i>
		Winston Pitts	<i>Revvng up a Designed Copper Nitrite Reductase Using Non-Natural Heterocycles</i>
		Raphael E.F. DePaiva	<i>On the Biology of Werner's Complex</i>
14:00	16:00	Annette Rompel	<i>Interweaving disciplines to advance chemistry: Applying polyoxometalates in biology</i>
14:30	16:30	Matt Allen	<i>Europium-Containing Contrast Agents for Magnetic Resonance Imaging</i>
15:00	17:00	Pernilla Wittung-Stafshede	<i>Role of copper chaperone Atox1 in cancer</i>
15:30	17:30	BREAK	

July 21, 2021

Session Chairs: *Andy Borovik and Debbie Crans*

GMT	Local Time	Speaker	Title
16:00	12:00 (NY)	Kara Bren	<i>Mini-Enzymes for Fuel Production and Small-Molecule Activation</i>
17:00	13:00	Liviu Mirica	<i>Novel Theranostic Agents for Alzheimer's Disease</i>
18:00	14:00	Magda Rowińska-Żyrek	<i>The bioinorganic secrets of antimicrobial peptides</i>
18:30	14:30	Eva Freisinger	<i>New features of plant metallothionein 3 forms</i>
19:00	15:00	Justin Wilson	<i>Chelation Strategies for Therapeutically Useful Alpha-Emitting Radionuclides</i>
19:30	15:30	Dan Suess	<i>Postbiosynthetic Modification of Nitrogenase Cofactors</i>
20:00	16:00	BREAK	

July 21, 2021

Session Chairs: *Liliana Quintanar and Alison Butler*

GMT	Local Time	Speaker	Title
20:30	16:30 (NY)	Ivan Castillo	Benzimidazole-based Ni, Co and Mn cubanes as water oxidation Catalysts
21:00	17:00	Ana C. Garcia-Alvarez	<i>Synthesis and Characterization of Benzimidazole Based Mn, Co, Ni Based Cubanes Bioinspired in the Active Site of Photosystem II</i>
		Mark Reynolds	<i>Studies of FixL from S. meliloti Reveal the Importance of a Conserved Salt Bridge in the Oxygen Sensing Mechanism</i>
		Marie Zoepfl	<i>Heparin Sulfate Targeting for Polynuclear Platinum Antiviral Activity</i>
		Martin E. Tovar-Ramirez	<i>Copper Coordination and Metal Induced aggregation of the Eye Lens Protein bB2-Crystallin</i>
		Jonathan Szuster	<i>Tuning Electron Transfer parameters by engineering a metal center in a non native protein scaffold</i>
		Santiago Rostán	<i>New potential anti T. cruzi agents: metal complexes of coumarin-thiosemicarbazone hybrid ligands</i>
		Kate Kostenkova	<i>Speciation as a tool to demystify the complexity of the biological polyoxovanadate chemistry</i>
		Gonzalo Scalese	<i>Exploring Molecular and Cellular Targets of Vanadium Compounds Against Trypanosoma Cruzi</i>
Victor Sosa Alfaro	<i>Elucidating Electron Storage and Distribution within the Pentaheme Scaffold of NrfA</i>		
22:30	18:30	Elene Pereira Maia	<i>Metal synthetic nucleases as anticancer drugs: copper complexes with hydroxyanthraquinones and N-heterocyclic ligands</i>
23:00	19:00	Zijian Guo	<i>Addressing the challenges of clinical platinum anticancer drugs</i>
23:30	19:30	BREAK	

July 22, 2021

Session Chairs: *Hugh Harris and Kazuya Kikuchi*

GMT	Local Time	Speaker	Title
00:00	8:00 (Beijing)	Paul Donnelly	<i>Theragnostics with Metal Complexes: Diagnosis and therapy of cancer and Motor Neuron Disease</i>
01:00	9:00	Marie Heffern	<i>Redefining metal-associated biomarkers in obesity-associated metabolic dysfunction</i>
01:30	9:30	Johannes Kargas	<i>Re(I) Tricarbonyl Complexes as Coordinate Covalent Inhibitors for the SARS-CoV-2 Main Protease</i>
		Chenyuan Wang	<i>Bismuth Siderophore Antibiotic Conjugate Combating Antimicrobial Resistance</i>
		Sumayah Asiri	<i>The Role of Cu Metabolism in the cis-platin sensitive and resistant ovarian cancer cells</i>
		Nicolas Bernier	<i>Inorganic Nanomaterials for Boron Delivery</i>
		Liam Eade	<i>Binding of Ru Piano Stool Complexes to ATG8 Family Proteins</i>
02:30	10:30	Marty Kirk	<i>Bioelectrochemical Hypoxia-activated Co(III) Compounds</i>
03:00	11:00	Rachel Codd	<i>Molybdenum Cofactor Sulfuration and Formal Hydride Transfer in Molybdoenzymes</i>
03:30	11:30	Somdatta Ghosh Dey	<i>A simple technology for metalloenzyme inhibitor discovery</i>
04:00	12:00	Somdatta Ghosh Dey	<i>Reactive Intermediates in Substrate Oxidation by Metal Amyloid Complexes relevant to Alzheimer's Disease</i>
04:00	12:00	BREAK	

July 22, 2021

Session Chairs: *Mi Hee Lim and Seung Jae Lee*

GMT	Local Time	Speaker	Title
04:30	12:30 (Beijing)	Yunho Lee	<i>The Mechanism of the CODH Reaction for CO₂ Conversion to CO at a Single Nickel Center</i>
05:00	13:00	Wei Xia	<i>Inhibition of SARS-CoV-2 main protease by metallodrugs</i>
05:30	13:30	Leela Ruckthong	<i>Structural and Spectroscopic Evidence Identifying a Pb(II) Binding Site in the Coiled Coil Region of the Human Line-1 ORF1p</i>
6:00	14:00	SK Amanullah	<i>The Role of Porphyrin Peripheral Substituents in Determining the Reactivities of Ferrous Nitrosyl Species</i>
		Paramita Saha	<i>Electrocatalytic Reduction of Nitrogen to Hydrazine Using a Trinuclear Nickel Complex</i>
		Fearghal Walsh	<i>Pyridinecarbothioamide Derived Cationic Complexes Which Target Mitochondria of Cancer Cells</i>
		Ana Luisa De Sousa-Coelho	<i>Recent advances into Vanadium and Melanoma</i>
6:30	14:30	Daniela Valensin	<i>Structural insights into copper interaction with polyphenols and amyloid beta peptides</i>
7:00	15:00	Anne Duhme-Klair	<i>Siderophore-catalyst Conjugates: Design and Applications</i>
07:30	16:00	Pecoraro and Harris	Closing Remarks