

# Scientific Program

## IX. Molybdenum & Tungsten Enzymes Conference 2015

Balatonfüred, Hungary

September 06 - 11

### Sunday, September 6

16:00	<b>Registration</b>
18:30	<b>Dinner</b>
19:45	<b>Welcome</b> (Rubin Hall) <b>Günter Schwarz</b> – University of Cologne, Germany
	<b>Plenary talk 1</b>
	Chair: <b>Sharon Burgmayer</b> – Bryn Mawr College, USA
	<b>Maria J. Romao</b> – Universidade Nova de Lisboa, Portugal Aldehyde Oxidases in Drug Metabolism and Biotransformations
21:00	<b>Reception</b> – Wine Tasting

## Monday, September 7

	Session 1 (Rubin hall) <b>DMSOR family of enzymes</b>
	Chair: <b>Jose J.G. Moura</b> – Universidade Nova de Lisboa, Portugal
08:30	<b>Joel Weiner</b> – University of Alberta, Canada Molybdenum Cofactor Diversity and Protein Fold Design Highlight the Importance of Pyranopterin Coordination in Substrate Reactivity
09:00	<b>Johann Heider</b> – Philipps-Universität Marburg, Germany Oxygen-independent hydrocarbon hydroxylation reactions by molybdenum enzymes: ethylbenzene dehydrogenase and family
09:30	<b>Gary Sawers</b> – Martin-Luther University Halle-Wittenberg, Germany The numerous nitrate reductases of the obligate aerobe <i>Streptomyces coelicolor</i>
	<b>Short talk</b>
10:00	<b>Justin G. Fedor</b> – University of Alberta, Canada Proton Transfer and Quinol Oxidation in <i>Escherichia coli</i> Nitrate Reductase
10:20	<b>Coffee break</b> (Borostyán Hall)
	Session 2 (Rubin Hall) <b>Formate dehydrogenases</b>
	Chair: <b>Silke Leimkühler</b> – University of Potsdam, Germany
10:50	<b>Judy Hirst</b> – Medical Research Council, Cambridge, United Kingdom Reversible interconversion of CO <sub>2</sub> and formate by tungsten- and molybdenum-containing formate dehydrogenases
11:20	<b>Russ Hille</b> – University of California, Riverside, USA Spectroscopic and Mechanistic Studies of the NAD <sup>+</sup> -dependent formate dehydrogenase from <i>Ralstonia eutropha</i> .
11:50	<b>Frank Sargent</b> – University of Dundee, United Kingdom Formate hydrogenlyases: enzymes of the past, enzymes of the future
	<b>Short talks</b>
12:20	<b>Arnau Bassegoda</b> – Medical Research Council, Cambridge, United Kingdom Elucidating the role of active site residues in <i>Escherichia coli</i> formate dehydrogenase-H by site directed mutagenesis

12:40	<b>Tobias Hartmann</b> – University of Potsdam, Germany Active Site Residues involved in Formate Oxidation and Nitrate Reduction Catalyzed by Formate Dehydrogenase of <i>Rhodobacter capsulatus</i>
13:00	<b>End of session</b>
13:15	<b>Lunch</b>
	<b>Session 3</b> (Rubin Hall) <b>Tungsten enyzmes</b>
	Chair: <b>Fred Hagen</b> – Delft University of Technology, Netherlands
14:15	<b>José Moura</b> – Universidade Nova de Lisboa, Portugal Periplasmic nitrate reductase and formate dehydrogenase
14:45	<b>Peter-Leon Hagedoorn</b> – Delft University of Technology, Netherlands Tungsten containing aldehyde ferredoxin oxidoreductases as part of a biocatalytic carboxylic acid hydrogenation system
15:15	<b>Simona G. Huwiler-Fischer</b> – Albert-Ludwigs-University of Freiburg, Germany Structure and function of a tungsten-containing benzoyl-CoA reductase
	<b>Short talk</b>
15:45	<b>Martin Culka</b> – University Bayreuth, Germany Anaerobic benzoyl-CoA aromatic ring reduction by BamB-I - computational mechanistic study
16:05	<b>Poster Session 1 and Coffee break</b> (Borostyán Hall) The <i>Scientific Advisory Board</i> will select 5 posters for a flash presentation on Tuesday evening. Preparing a 7 min presentation in advance is recommended.
18:30	<b>Dinner</b>
20:00	<b>Plenary talk 2</b> (Rubin Hall)
	Chair: <b>Lance Seefeldt</b> – Utah State University, USA
	<b>Brian M. Hoffman</b> – Northwestern University, Evanston, USA Nitrogenase: History; Molybdenum; Mechanism
21:00	<b>Bar</b>

## Tuesday, September 8

	Session 4 (Rubin Hall) <b>Electrochemistry of Mo enzymes</b>
	Chair: <b>John H. Enemark</b> – University of Arizona, Tucson, USA
08:30	<b>Vincent Fourmond</b> – CNRS & Aix-Marseille Université, France What can we learn about nitrate reductases using protein film voltammetry?
09:00	<b>Paul Bernhardt</b> – University of Queensland, Brisbane, Australia Molybdenum Enzyme Electrochemical Communicatio
	<b>Short talks</b>
09:30	<b>Barbara Schoepp-Cothenet</b> – CNRS & Aix-Marseille University, France The electrochemical properties of the molybdenum cofactor in bis-PGD enzymes resemble those of quinones
9:50	<b>Ulla Wollenberger</b> – <b>University of Potsdam, Germany</b> Effective bioelectrocatalysis of molybdoenzymes and biosensor application
10:10	<b>Coffee break</b> (Borostyán Hall)
	Session 5 (Rubin Hall) <b>Model compounds</b>
	Chair: <b>Marty Kirk</b> – The University of New Mexico, Albuquerque, USA
10:50	<b>Partha Basu</b> – Duquesne University, Pittsburgh, USA Synthesizing Molybdopterin Using Regioselective Condensation
11:20	<b>Carola Schulzke</b> – Ernst-Moritz-Arndt-Universität Greifswald, Germany Fine-tuning molybdenum dithiolene chemistry for structural and functional MoCo models
11:50	<b>Sharon Burgmayer</b> – Bryn Mawr College, USA Exploring Molybdenum Pterin-Dithiolene Reaction Chemistry
	<b>Short talks</b>
12:20	<b>Mohsen Ahmadi</b> – Ernst-Moritz-Arndt-Universität Greifswald, Germany On the way to phosphate substituted dithiolene complexes as models for the active site of molybdenum and tungsten dependent oxidoreductases

12:40	<b>Emmanuel Oheix</b> – Aix-Marseille Université, Marseille, France Synthesis, characterization, and catalytic activity of 2-hydroxo and 2-mercaptopyridine-N-oxide complexes of molybdenum VI
13:00	<b>End of session</b>
13:15	<b>Lunch</b>
	Session 6 (Rubin Hall) <b>Model compounds</b>
	Chair: <b>Partha Basu</b> – Duquesne University, Pittsburgh, USA
14:15	<b>Ralf R. Mendel</b> – Technical University Braunschweig, Germany The final step in molybdenum cofactor biosynthesis in plants
14:45	<b>Silke Leimkühler</b> – University of Potsdam, Germany The biosynthesis of the molybdenum cofactor in bacteria
15:15	<b>Kenichi Yokoyama</b> – Duke University Medical Center, Durham, USA Capturing a Cryptic Biosynthetic Intermediate Reveals the Mechanism of Pyranopterin Ring Formation in Molybdenum Cofactor Biosynthesis
	<b>Short talks</b>
15:45	<b>Fabio Amadei</b> – University of Zurich, Switzerland Interaction between Moco and the <i>moaA</i> Moco RNA motif from <i>E. coli</i>
16:05	<b>Poster Session 2 and Coffee break</b> (Borostyán hall)
18:30	<b>Dinner</b>
19:45	<b>Selected Poster Talks</b>
	Chair: <b>Markus Ribbe</b> – University of California, Irvine, USA
	<b>Talks</b> will be selected on Monday's poster session and announced before the Planary talk 1. Speakers will have the opportunity to present 7 min talks + 5 min discussion
21:00	<b>Bar</b>

## Wednesday, September 9

	Session 7 (Rubin Hall) <b>Spectroscopy and Computational Studies</b>
	Chair: <b>Brian M. Hoffman</b> – Northwestern University, Chicago, USA
08:30	<b>Marty Kirk</b> – The University of New Mexico, Albuquerque, USA Unusual Atom Transfer Type Chemistry in Pyranopterin Molybdenum Enzymes
09:00	<b>Graham George</b> – University of Saskatchewan, Canada A Holistic view of Mo and W Enzymes: Combining X-ray Spectroscopy, Computational Chemistry and Structural Studies
09:30	<b>Matthias Ullmann</b> – University Bayreuth, Germany Simulating Charge Transfer in Protein Complexes
	<b>Short talk</b>
10:00	<b>Maciej Szaleniec</b> – Jerzy Haber Institute, Polish Academy of Sciences, Poland QM:MM study of the ethylbenzene dehydrogenase reaction mechanism
10:20	<b>Coffee break</b> (Borostyán Hall)
	Session 8 (Rubin Hall) <b>Nitrogenase and FeMoCo</b>
	Chair: <b>Russ Hille</b> – University of California, Riverside, USA
10:50	<b>Lance Seefeldt</b> – Utah State University, USA Insights into the Nitrogenase Mechanism
11:20	<b>Markus Ribbe</b> – University of California, Irvine, USA CO-reduction by nitrogenase
11:50	<b>Oliver Einsle</b> – Albert-Ludwigs-University of Freiburg, Germany Crystallography of Mo- and W-proteins: What you see ... and what you think you see
12:20	<b>Yilin Hu</b> – University of California, Irvine, USA The function of NifB in nitrogenase M-cluster assembly
13:00	<b>Lunch</b>

14:00	<b>Business Meeting</b> (Onyx Room)
14:30	<b>Departure</b> to Excursion, Balatonfüred Harbor
15:00	<b>Boat Cruise</b> & Wine Tasting
18:30	<b>Dinner</b>
19:45	<b>Plenary talk 3</b> (Borostyán Hall)
	Chair: <b>Günter Schwarz</b> – University of Cologne, Germany
	<b>Ashley I. Bush</b> – The Florey Institute, University of Melbourne, Australia Metals in Neurodegenerative Disease
21:00	<b>Bar</b>

## Thursday, September 10

	Session 9 (Rubin hall) <b>Sulfite oxidase family</b>
	<b>Chair:</b> Katrin Schrader – University of Cologne, Germany
08:30	<b>Courtney Sparacino-Watkins</b> – School of Medicine, University of Pittsburgh, USA The role of enzymatic nitrite reduction to NO by mARC-2 in pulmonary arterial hypertension.
	<b>Short talk</b>
09:00	<b>John H. Enemark</b> – University of Arizona, Tucson, USA Sulfite Oxidase: A Paradigm for the Mechanistic Complexities and Mysteries of Metallo-enzymes with Multiple Domains, Subunits and Cofactors
09:20	<b>Daniel Bender</b> – University of Cologne, Germany Mechanism of nitrite-dependent NO synthesis by sulfite oxidase
09:40	<b>Luisa Maia</b> – Universidade Nova de Lisboa, Portugal Nitrite reduction by molybdoenzymes: an ubiquitous function to generate signalling nitric oxide
10:00	<b>John Thomas</b> – Duquesne University, Pittsburgh, USA Protein Interactions of Mitochondrial Amidoxime Reducing Component Proteins in Kidney HEK-293 Cells
10:20	<b>Coffee break</b> (Borostyán hall)
	Session 10 (Rubin Hall) <b>Xanthine oxidase family</b>
	Chair: <b>Maria J. Romao</b> – Universidade Nova de Lisboa, Portugal
10:50	<b>Florian Bittner</b> – Technical University Braunschweig, Germany Insights into the final activation mechanism of molybdoenzymes of the xanthine oxidase family
11:20	<b>Enrico Garattini</b> – Istituto di Ricerche Farmacologiche "Mario Negri", Milano, Italy The molybdo-flavoenzyme aldehyde oxidase 4 controls mouse circadian rhythms, fat deposition and locomotor activity
	<b>Short talk</b>

11:50	<b>Alessandro Foti</b> – University of Potsdam, Germany Investigations of single nucleotide polymorphisms (SNP) in the active site of human aldehyde oxidase
12:10	<b>Catarina Coelho</b> – Universidade Nova de Lisboa, Portugal Structural Determinants of Substrate Specificity in Mouse Aldehyde Oxidases Isoforms
12:30	<b>Yuko Kawaguchi</b> – Nippon Medical School, Tokyo, Japan The role of Asp428 on the FAD reactivity in rat xanthine dehydrogenase
13:15	<b>Lunch</b>
	Session 11 (Rubin Hall) <b>Medical Aspects</b>
	Chair: <b>Ralf Mendel</b> – Technical University Braunschweig, Germany
14:15	<b>Bernd Schwahn</b> – Central Manchester University Hospitals, United Kingdom Efficacy and safety of cyclic pyranopterin monophosphate substitution in severe molybdenum cofactor deficiency typeA
14:45	<b>Bernd Clement</b> – Kiel University, Germany Novel aspects of the human molybdenum containing enzyme mARC
15:15	<b>Abdel A. Belaidi</b> –University of Melbourne, Australia Sulfite oxidation in humans: from basic metabolism to therapy
15:45	<b>Jennifer Schneider</b> – Kiel University, Germany mARC and its potential role in prevention of cardiovascular disease
16:05	<b>Poster Session 3 and Coffee break</b> (Borostyán hall)
18:30	<b>Departure</b> to Conference Dinner
19:00	Visit <b>Tihany</b> Monastery
19:30	<b>Conference Dinner</b>
23:00	<b>Return</b> to Hotel

**Friday, September 11**

	<b>Departure</b>
9:00	Shuttle bus to <b>Vienna</b> airport
9:15	Shuttle bus to <b>Budapest</b> airport