

# 3rd BioXAS Study Weekend “Metalloproteomics”

## A satellite meeting of BSR2007

Synchrotron-Soleil, Saint-Aubin, France  
10-11 August 2007

### PROGRAMME

Registration at Synchrotron-Soleil  
10 August: 8:30-9:15

## 10 August 2007

09:15 – 09:30 Welcome  
*Michel Van der Rest (Synchrotron-Soleil, France)*

09:30 – 10:00 Soleil: status and the integrated biology programme  
*Roger Fourme (Synchrotron-Soleil, France)*

### **SESSION 1: Impact of 3rd generation synchrotrons on BioXAS : advanced beamlines on Synchrotron-Soleil, Canadian Light Source, Petra III and Diamond Light Source.**

10:00 – 10:30 Metalloproteins & BioXAS programme at Soleil  
*Isabella Ascone (Synchrotron-Soleil, France)*

10:30 – 11:00 The BioXAS project at CLS, spectroscopic imaging and related research.  
*Gosia Korbas (University of Saskatchewan, Canada)*

11:00-11:15 **Coffee break**

11:15 – 11:45 Facilities for Complementing X-ray Macromolecular Crystallography:  
Present and Future  
*Michele Cianci (EMBL Hamburg Outstation, Germany)*

11:45 – 12:15 Opportunities for BioXAS at the high resolution spectroscopy beamline at  
Diamond  
*Sofia Diaz-Moreno (Diamond Light Source, UK)*

12:15 - 13:45 **Lunch at Synchrotron Soleil restaurant**

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### **SESSION 2: Biological challenges to select and prepare relevant Metalloproteins samples**

- 13:45 – 14:30** Metalloproteomics : problems, challenges and joys (review)  
*Samar S. Hasnain (Daresbury Laboratory, UK)*
- 14:30 – 15:00** Metal Environment and Structural Genomics  
*Wladek Minor (University of Virginia, USA)*
- 15:00 – 15:30** Search of metalloproteins in proteomes: a bioinformatic approach  
*Claudia Andreini (CERM, University of Florence, Italy)*
- 15:30 – 16:00** Metalloprotein expression and identification: experience at Genomic Sciences Center (RIKEN)  
*Seiki Kuramitsu (RIKEN SPring-8 Center, Japan)*
- 16:00 – 16:15** **Coffee Break**

### **SESSION 3: Metalloproteins in solution: BioXAS structural determinations at chemical equilibrium or during a chemical reaction.**

- 16:15 – 16:45** Redox activity of biomimetic Mn complexes: results from time resolved x-ray absorption spectroscopy  
*James Penner-Hahn (University of Michigan, USA)*
- 16:45 – 17:15** The icing on the cake – combining x-ray absorption spectroscopy with protein crystallography  
*Wolfram Meyer-Klaucke (EMBL Hambourg Outstation, Germany)*
- 17:30 – 18:15** **Visit to Synchrotron-Soleil Facilities**
- 18:15 – 19:30** **Poster session**
- 19:30 – 21:30** **Social dinner**

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# 11 August 2007

### SESSION 4: Combined techniques and high throughput structure determination (PX, single crystal BioXAS and other techniques)

- 09:30 – 10:15** Structural Biology, Genomics, Metalloproteins & BioXAS at SSRL (review)  
*Britt Hedman (Stanford Synchrotron Radiation Laboratory, USA)*
- 10:15 -10:45** Multiple Scattering XAFS Studies of Heme Proteins  
*Peter Lay (The University of Sydney, Australia)*
- 10:45 – 11:15** Mn complex in PS II  
*Vittal Yachandra (Lawrence Berkeley National Laboratory, USA)*
- 11:15 -11:30** **Coffee Break**
- 11:30 – 12:00** Atomic resolution structures and BioXAS - single crystal at Daresbury  
*Richard W. Strange (Daresbury Laboratory, UK)*
- 12:00 – 12:30** X-ray Absorption Fine Structure studies of Zn<sup>2+</sup> binding sites in charge translocating membrane protein complexes  
*Lisa Giachini (University of Bologna, Italy)*
- 12:30 – 14:00** **Lunch at Synchrotron Soleil restaurant**

### SESSION 5: Theoretical advances and edge/XANES analysis

- 14:00 – 14:30** Recent advances in the calculation of X-ray Absorption Spectra (XAS) and their relevance for the extraction of structural and electronic parameters in systems of biological interest  
*Calogero Natoli (INFN-Laboratori Nazionali Frascati, Italy)*
- 14:30 – 15:00** Theoretical simulations and analysis of BioXAS with only structural parameters  
*John J. Rehr (University of Washington, USA)*
- 15:00 -15:15** **Coffee Break**
- 15:15 – 15:45** Time-dependent Density Functional Calculations of XAS Pre-edges  
*Serena DeBeer George (Stanford Synchrotron Radiation Laboratory, USA)*
- 15:45 – 16:15** K $\beta$ -detected high resolution XANES in models of catechol oxygenase.  
*Ana Mijovilovich (Utrecht University, The Netherlands)*
- 16:15 – 17:30** **Poster session**