

ISDSB 2010 – 3rd International Symposium on Diffraction Structural Biology

May 25-28th, 2010, Auditorium Pierre
Lehmann, LAL, Bldg 200
Paris-Sud/XI University, Orsay, France

Programme

Tuesday, May 25th

12:00 *Registration* Auditorium Pierre Lehmann, LAL, Bldg. 200 Paris Sud/XI University,
Orsay, France

14:00 – 14:30 **Welcome**

M. Van der Rest, SOLEIL (SOLEIL DG), representatives of Region Ile de France
and Paris-Sud University & J. Takahara (Minister Plenipotentiary, Embassy of
Japan in France)

14:30 – 15:30 **Opening lecture**

Chair: Roger Fourme

What we have learnt from the structures of ribosome.
Venki Ramakrishnan, MRC LMB Cambridge, UK

15:30 – 16:00 *Coffee break*

16:00 – 18:00 **S1. Electron microscopy, X-ray imaging, tomography**

Chair: Wolfgang Baumeister

Electron cryo-tomography of eukaryotic flagella and cilia.
Takashi Ishikawa, ETH Zurich, Switzerland

Electron microscopy of membrane proteins - from atomic structure to in situ
arrangement. Werner Kühlbrandt, MPI, Frankfurt, Germany

Imaging cells using correlated fluorescence and x-ray tomography.
Carolyn Larabell, UCSF, San Francisco, CA, USA

Electron and X-ray tomography of the malaria parasite, *P. falciparum*.
Leann Tilley, La Trobe U., Melbourne, Australia

18:00 – 18:30 *Transfer to Synchrotron SOLEIL (Saint Aubin) by bus*

18:30 – 20:30 *Welcome party at Synchrotron SOLEIL*

Wednesday, May 26th

09:00 – 09:45 **Plenary talk**

Chair: Ian Wilson

Synchrotrons, high throughput crystallography and discovery of new medicines:
drugging the undruggable. Tom Blundell, Cambridge U., UK

09:45 – 10:15 *Coffee break*

10:15 – 12:45 S2. Drug and vaccine design

Chair: Tom Blundell

Structure-based vaccine design. Phillip Dormitzer, Novartis, Cambridge, MA, USA

Drug discovery facilitated by biophysical methods. Michael Hennig, Hoffmann-La Roche, Basel, Switzerland

Chemogenomic profiling in structure-based drug design: what are optimal ligandbinding parameters for a given target? Gerhard Klebe, Marburg U., Germany

Structural genomics of the human G-protein coupled receptor family. Raymond Stevens, Scripps Research Institute, La Jolla, CA, USA

Drug design of hematopoietic prostaglandin D synthase inhibitors based on high resolution X-ray crystallography. Yoshihiro Urade, Osaka Bioscience Institute, Osaka, Japan

13:00 – 14:30 Lunch at University Restaurant – Bldg 230

14:30 – 16:00 S3. Protonation States

Chair: John Helliwell

Protons in proteins. Matthew Blakeley, ILL, Grenoble, France

Diisopropyl fluorophosphatase: from protonation states to protein engineering. Julian Chen, Institute of Biophysical Chemistry, Goethe University, Frankfurt, Germany

Histidine protonation states in a human hemoglobin. Yukio Morimoto, Research Reactor Inst., U. Kyoto, Kumatori, Osaka, Japan

16:00 – 16:30 Coffee break

16:30 – 18:00 S4. Large Bio Molecules

Chair: Jack Johnson

Seeing the structural organization of the actin cytoskeleton at the lamella by in situ cryo-electron tomography. Dorit Hanein, Burnham Inst. for Medical Research, La Jolla, CA, USA

3D architecture and allosteric changes for cell entry of the envelope glycoprotein shell of Chikungunya virus. Felix Rey, Institut Pasteur, Paris, France

Ribosome dynamics and tRNA movement as visualized by time-resolved electron cryomicroscopy. Holger Stark, MPI, Göttingen, Germany

18:00 – 18:45 Plenary talk

Chair: Wayne Hendrickson

Exploiting the anisotropy of anomalous scattering boosts the phasing power of SAD and MAD experiments. Gérard Bricogne, Global Phasing Ltd, Cambridge, UK

19:00 Transfer for a boat trip with dinner on Seine

20:00 – 22:30 Conference Dinner on Seine

Thursday May 27th

08:45 – 09:30 **Plenary talk** Chair: Gérard Bricogne

Small angle X-ray scattering of biological macromolecules.
Dmitri Svergun, EMBL, Hamburg, Germany

09:30 – 09:50 *Coffee break*

09:50 – 11:20 **S5. Membrane Proteins**
Chair: Gebhard Schertler

Crystal structures of the autotransporter EspP before and after passenger cleavage reveals a novel outer membrane cleavage. Susan Buchanan, NIDDK, Bethesda, MD, USA

Structure of photosystem complex around oxygen-evolving Mn₄ OxCa-cluster. Nobuo Kamiya, Osaka City U., Osaka, Japan

Molecular basis of the alternating access model of membrane transport by the sodium-hydantoin transporter, Mhp1. Alex Cameron, MPL Diamond, Chilton, UK

11:20 – 11:40 *Coffee break*

11:40 – 13:15 **S6. Protein Structure/Function**
Chair: Nori Yasuoka

Allosteric control of nuclear receptors dimerization. Dino Moras, IGBMC, CNRS-INSERM-ULP, Strasbourg, France

Glutamate dehydrogenase: structure, allostery, evolution, and role in insulin homeostasis. Thomas J. Smith, Danforth Plant Science Center, Saint Louis, MI, USA

Structures, regulation and evolution of glutamate synthases. Maria Vanoni, U. of Milano, Milano, Italy

13:15 – 14:30 *Lunch at University Restaurant – Bldg 230*

14:30 – 15:00 *Transfer to Synchrotron SOLEIL by bus*

15:00 – 19:00 Poster session I and commercial exhibitors

Visit of the facility

Friday May 28th

08:45 – 09:30 **Plenary talk**

Chair: Claudio Luchinat

Structure-inspired functional discovery for a family of novel ion channels. Wayne Hendrickson, Columbia U., New York, USA

09:30 – 09:50 *Coffee break*

09:50 – 12:00 **S7. Coupling NMR/XRD, X-ray technologies**

Chair: Nori Sakabe

Small angle X-ray data and paramagnetism-based NMR restraints are highly complementary in defining the conformational space sampled by flexible two-domain proteins. Claudio Luchinat, CERM, U. of Florence, Italy

Microbeam macromolecular crystallography and reduced radiation damage. Robert Fischetti, APS, Argonne, USA

High-pressure macromolecular crystallography status and applications. Eric Girard, IBS, Grenoble, France

The future of micro- and nano-diffraction of membrane protein samples. Gebhard Schertler, Paul Scherrer Institute, Villigen, Switzerland

Provision for hot topic

12:00 – 13:15 Poster session II (LAL, Salle Bleue – Bldg 200)

13:15 – 14:30 *Lunch at University Restaurant – Bldg 230*

14:30 – 15:15 **Plenary talk** Chair: Matthew Blakeley

Neutrons in diffraction structural biology making the best use of neutrons. Ichiro Tanaka, Ibaraki U., Japan

15:15 – 15:45 *Coffee break*

15:45 – 17:15 **S8. Structural Genomics**

Chair: Dino Moras

Structural genomics and the expanding protein universe. Ian Wilson, JCSG, Scripps Research Inst., La Jolla, CA, USA

Non-protein components of protein structures and other biomedical aspects of structural genomics. Wladek Minor, MCSG, CSGID, U. of Virginia, Charlottesville, VA, USA

Family wide structural and functional analysis of the human proteome. Stefan Knapp, SGC, U. of Oxford, Oxford, UK

17:15 - 18:00 **Plenary talk**

Chair: Leann Tilley

Electron cryomicroscopy: from molecules to systems. Wolfgang Baumeister, MPI Martinsried, Germany

18:00 – 18:15 *Closing Ceremony*

Poster Presentations

SESSION I

- PO-SI-01** Structural Studies and Sequencing of the Giant Haemoglobin from Glossoscolex Paulistus
Bachega, J.F.R.,
- PO-SI-02** Ultrastructural Organization of Budding Yeast Septin Filaments Both *in vitro* and *in situ*, Analyzed by Electron Microscopy
Bertin A.
- PO-SI-03** High Resolution Crystal Structure of the *E.coli* Malto porin
Blaise M.
- PO-SI-04** Bacteriophage T5, a Model System for Investigating the Assembly Pathway of a T=13 Capsid
Boulanger P.
- PO-SI-05** Structural and functional comparison between Hepatitis C Virus JFH1 and J6 polymerases
Caillet-Saguy C.
- PO-SI-06** Structure-function Study of Metal-dependent Fructose-1,6-bisphosphate Aldolases: Catalysis and Drug-design
Coinçon M.
- PO-SI-07** 5-hydroxy-5-methylhydantoin DNA Containing Lesion: a Molecular Trap for DNA Glycosylases
Coste F.
- PO-SI-08** Structure Analysis of Group I Plant Nucleases
Dohnalek J.
- PO-SI-09** Crystal Structure of a Nucleocapsid-like Nucleoprotein-RNA Complex of Respiratory Syncytial Virus
Duquerroy S.
- PO-SI-10** Structural Basis of Targeting of the Human Cytokine CSF-1 by the Viral Oncoprotein BARF1
Elegheert, J.
- PO-SI-11** Structural Insights and *ab initio* Sequencing within the DING Proteins Family
Elias M.
- PO-SI-12** Time-Resolved Crystal Structure Analysis of Mn(II) Dependent Hydrolysis Reaction of ADP-Ribose Pyrophosphatase from *Thermus thermophilus* HB8
Furuike Y.

PO-SI-13 Conformational Changes of Hepatitis C Virus Polymerase in Solution: Opening and Closure, or SAXS Artifact?

Harrus D.

PO-SI-14 The Structural Chemistry and Structural Biology of Coloration in Marine Crustacea

Helliwell J.R.

PO-SI-15 The Ultra High-resolution X-ray Structure of Bovine H-protein at 0.79 Å; the Crystals Grown in Microgravity Environment

Higashiura A.

PO-SI-16 Structural and Functional Study of a Vitamin D Receptor Mutant that Responds Selectively to Gemini Ligands

Huet T.

PO-SI-17 Crystal Structure of the Glycosylated Form of Interleukin-23.

Ikemizu S.

PO-SI-18 Structural and Functional Studies of the Sarcoplasmic Reticulum Ca²⁺-ATPase

Jurková I.

PO-SI-19 Structural Basis for Histidine Mediated Vitamin D Receptor Agonistic and Antagonistic Mechanisms of (23S)-25-dehydro-1α-hydroxyvitamin D₃ 26,23-lactone

Kakuda S.

PO-SI-20 X-ray Crystal Structure Analysis of Reaction Intermediate of Copper Amine Oxidase from *Arthrobacter globiformis*

Kataoka M.

PO-SI-21 A Preliminary Neutron Crystallography on the Trypsin-bovine Pancreatic Trypsin Inhibitor Complex

Kawamura K.

PO-SI-22 Catalysis in the Nitrilase Superfamily Enzymes; a Catalytic Triad or Tetrad?

Kimani S.

PO-SI-23 Crossroads Structural Study of the Architecture of Rap1 Protein Involved in Telomere Stability

LeDu M.H.

PO-SI-24 A Unique Secondary Structure Switch Controls Constitutive Gene Silencing by Retinoic Acid Receptor

le Maire A.

PO-SI-25 Anesthetic Gas Xenon and Nitrous Oxide: Same Physiological Target and Same Binding Site in Proteins

Marassio G.

PO-SI-26 Crystallographic Structure of a Ribosomal RNA Methylase Involved in Bacterial resistance to Aminoglycosides

Mechulam Y.

PO-SI-27 Structure of Nicotinic Acetylcholine Receptor in the Desensitized States

Nishino Y.

- PO-SI-28** Substituted Pyrazolopyrimidines as Potent, Selective and CNS Active Inhibitors of CK1d and CK1e
Ohren J.F.
- PO-SI-29** Purine Nucleoside Phosphorylase from *Schistosoma mansoni* in Complex with Ribose-1-Phosphate
Pereira H.M.
- PO-SI-30** The Intriguing Quinone Reducing Site (Qi) of the Cytochrome *b6f* Complex
Picot D.
- PO-SI-31** Structural Studies of Glycosidase with High Specificity Towards the Blood Group B Antigen
Ponchel G.
- PO-SI-32** Azide and Cyanide Have Different Inhibition Modes in Urate Oxidase
Prangé T.
- PO-SI-33** Crystal Structure of Stable Protein, CutA1, from a Psychrotrophic Bacterium *Shewanella* sp. SIB1
Takano K.
- PO-SI-34** Structural Studies of Transcription Factor IIIC
Taylor N.M.I.
- PO-SI-35** Three-dimensional Structure of HSP104, a Yeast Prion-remodeling Machine
Tsai F.T.F.
- PO-SI-36** Kinetics of Hepatitis B Virus Core Assembly by Time-resolved Solution X-ray Scattering
Tsuruta H.
- PO-SI-37** Structural Studies of MobR, the 3-hydroxybenzoateresponsive Transcriptional Regulator for the 3-hydroxybenzoate Hydroxylase Gene of *Comamonas Testosteroni* KH122-3s
Yamaguchi H.
- PO-SI-38** NADPH-free and -bound Structures of Conjugated Polyketone Reductase C2 (CPR-C2) from *Candida Parapsilosis* IFO 0708
Yamamura A.
- PO-SI-39** Water-mediated Crystal Transformations of D-xylose Isomerase and Thaumatin
Yamamura S.
- PO-SI-40** Decreased Particle Size Explains Improved Protein Yield in E.coli expressed *Manihot esculenta* Hydroxynitrile Lyase Mutants
Yamane T.
- PO-SI-41** The Structural Basis of Serpin Polymerization
Yamasaki M.
- PO-SI-42** Structural Insights into the High Affinity Binding of Cardiac Glycosides to the Na⁺,K⁺-ATPase
Yamane L.

Poster Presentations

SESSION II

- PO-SII-01** Biomolecular Solution X-ray Scattering at the National Synchrotron Light Source
Allaire M.
- PO-SII-02** UV-based Automated Crystal Centering
Chavas Léonard M.G.
- PO-SII-03** High Pressure Cryocooling and Microcrystallography @ MacCHESS
English U.
- PO-SII-04** A New Paradigm for Macromolecular Crystallography Beamlines
Fourme R.
- PO-SII-05** Interactions of Biomacromolecules - Protein Surface Modifying Agents in Protein Crystallization
Hašek J.
- PO-SII-06** Upgrade of High-throughput Sample Exchange Robots PAM and Development of PAM/SPACE Reversible Cassettes
Hirakia M.
- PO-SII-07** High-precision and High-throughput Diffractometer System for Macromolecular Crystallography Beamlines at the Photon Factory
Igarashi N.
- PO-SII-08** The Cd-Te XPAD3S, a 2D Photon Counting Detector for High-Energy Applications.
Medjoubi K.
- PO-SII-09** Synchrotron Radiation Beamline for Macromolecular Assemblies Operated by the IPR at SPring-8
Nakagawa A.
- PO-SII-10** Correlated Single-crystal Spectroscopy and X-ray Crystallography at Beamline X26-C of the NSLS
Orville A.M.
- PO-SII-11** Research and Development of the Electron Beam Focusing System for a High Brightness X-ray Generator
Sakai T.
- PO-SII-12** The Role of Modern Home-lab X-ray Systems in Increasing Beamline Efficiency
Smith V.
- PO-SII-13** Improvement of Crystal Quality of Hematopoietic Prostaglandin D Synthase with Novel Inhibitors in Microgravity Environment
Takahashi S.

PO-SII-14 Lanthanoid Complexes as New Tools for X-ray Structure Determination of Biological Macromolecules: Application to Large Protein Complexes and Membrane Proteins.

Talon R.

PO-SII-15 Use of a 3 Circle Kappa Goniometer Goniostat for Structure Determination Using Anomalous Diffraction on PROXIMA 1.

Thompson A.

PO-SII-16 Automation at SLS Protein Crystallography Beamline X06DA: from Crystallization to Structure Determination

Wang M.

PO-SII-17 Semi-automated Protein Crystal Mounting Device for S-SAD Phasing and its Loop Implementation Tool

Watanabe N.

PO-SII-18 Fully Automated Data Collection and Processing System in the Photon Factory Macromolecular Crystallography Beamlines

Yamada Y.

PO-SII-19 The Structural Basis of Serpin Polymerization

Yamasaki M.