

SIG1: Macromolecular Crystallography

Reported Period: 2012-2013

Report Date: 3 June 2013

Reported by: Gerlind Sulzenbacher

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1. Introduction. (50 words max.)

The principal objectives of the Macromolecular Crystallography SIG are to support advances in macromolecular crystallographic research by both theoretical and experimental methods and their applications, and to represent and bring together researchers interested in these areas.

2. SIG web site:

SIG1 url: <http://www.afmb.univ-mrs.fr/SIG1>

3. Number of ECA individual members registered with the SIG according to (<http://www.xray.cz/eca/im-payment.htm>)

SIG1	Macromolecular Crystallography	158
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4. Existence of a SIG mailing list: No

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate)

SIG1 currently has 158 registered members (from <http://www.xray.cz/eca/eca-sig.asp?id=SIG1>), while meetings are normally attended by ~30 individuals. Several dozens of researchers are involved in SIG1 activities, especially in the organization of courses and workshops, but unfortunately they do not necessarily renew their ECA membership on a yearly basis.

6. List of MS organized by the SIG at the last ECM

MS 1 Protein crystallization and sample preparation
MS 2 MX at Synchrotron Sources, including X-FELs and time-resolved crystallography
MS 3 Getting the best data from your crystal(s)
MS 4 Phasing challenges. Bootstrapping from a poor start
MS 5 Advances in refinement and validation. Ligand chemistry
MS 6 Bioinformatics informs MX
MS 7 Pharmaceutical crystallography - Drug design: success and failures
MS 8 Membrane proteins
MS 9 EM and MX for viruses, assemblies and biological nano-machines
MS 10 Infection and Disease
MS 11 Frontiers in Structural Enzymology
MS 12 Molecular recognition

7. Prizes sponsored/coordinated

Title : IUCr Poster Prize at ECM27, Bergen

Prize : Three Prizes: Each a complimentary online access to all IUCr journals for one year, or volume of Int Tables for Crystallography.

Sponsor : IUCr

Eligibility : Best poster graduate/ undergrad student ; one each from FA1, FA2 & FA3

Selection Panel : Kamil Dziubek

Winning poster FA1 : Insulin Analogues for Insulin Receptor Studies and Medical Applications. Christopher J. Watson, YSBL, University of York, UK.

Title : RCSB PDB Poster Prize at ECM27, Bergen

Prize : Related educational book

Sponsor : Research Collaboratory for Structural Bioinformatics Protein Data Bank

Eligibility : Best student posters related to macromolecular crystallography

Selection Panel : Udo Heinemann (Max-Delbrück Center for Molecular Medicine, Berlin), Linda Shimon (Weizmann Institute of Science), and Ute Krengel (University of Oslo).

Winning poster : *Cardiotonic Steroids and the Na/K-ATPase*. Jonas Lindholt, Linda Reinhard, Poul Nissen, Centre for Membrane Pumps in Cells and Disease (PUMPkin) and Department of Molecular Biology and Genetics, Aarhus University, Denmark)

8. Past Activities other than Microsymposia at ECM

An important number of workshops and courses have been organized by individual SIG1 members, including CCP4 initiatives, EMBO training courses and other courses financed with European or national funds. Some of the activities have been sponsored by ECM or IUCr.

9. Future/Programmed Activities.

Currently SIG1 is actively organising a number of keynote lecture and microsymposia for the forthcoming ECM28 meeting in Warwick.

Keynote Lectures:

Manajit Hayer-Hartl, MPI Biochemistry Martinsried, Germany, Molecular chaperones for the folding, assembly and maintenance of RuBisCO

Wayne Hendrickson, University of Columbia, USA, Multi-crystal Native SAD Analysis of Macromolecular Structure

Sebastien Boutet, SLAC National Accelerator Laboratory, USA, X-ray FEL instrumentation for structure and dynamics of biomolecules

Marat Yusupov, IGBMC, Strasbourg, France, Crystal structure of eukaryotic ribosome

Microsymposia (Co-Chairs):

MS1 XFEL and time resolved crystallographic methods (John Helliwell, Victor Lamzin)

MS2 Multi-crystal techniques (Wayne Hendrickson, Sean McSweeney)

MS3 Hybrid approaches (SAXS, EM, etc + MX) (Bruno Kläholtz, Guillermo Montoya)

MS4 Advances in refinement, phasing and autobuilding (Michael Kokkinidis, Isabel Uson)

MS5 Structure and function of biomacromolecules (Marjolein Thunnissen, Gerlind Sulzenbacher)

MS6 Macromolecular assemblies (Marat Yusupov, Matthias Willmanns)

MS7 Membrane proteins (Elizabeth Carpenter, Martin Caffrey)

MS8 Cell signalling - interactions and allostery (Jacqueline Cherfils, Remy Loris)

MS9 Protein-nucleic acid complexes (Udo Heinemann, Elisabeth Sauer-Eriksson)

MS10 General interests of single molecule crystallography, both large and small (Thomas Schneider, Kirsten Christianen)

MS11 Twinning: problems and advantages (Loes Kroon-Batenburg, Pietro Roversi)

MS12 Radiation damage (Max Nanao, Arwen Pearson)

As for past activities, a large panel of workshops and courses are foreseen for the coming year. A specificity of SIG1 is the fact that sample preparation is an important part of structural biology and the theme of many courses goes well beyond crystallography. Many of the activities will be organised by INSTRUCT, <http://www.structuralbiology.eu/>, the network for structural biology in Europe.

10. Other matters.

The last annual meeting of SIG1 took place at ECM27 in Bergen. About 10 people attended the meeting and provided ideas and input for the forthcoming ECM28 to be held in Warwick. The next meeting of SIG1 will be held at the ECM28.

11. Brief annual activity report (100 words max.)

The main activity of SIG1 involves the organization of the microsymbiosia and keynote speakers for the individual European crystallographic meetings. The aim is to offer a wide variety of topics to structural biologists with a view to increase the attendance of our current and potential members at the annual meetings. In addition, individual members participate in organizing workshops and conferences of interest to European structural biologists.

12. List SIG officers, name and e-mail, and specify their main function in the SIG:

Chair: Keith Wilson, York, United Kingdom, keith@ysbl.york.ac.uk

Vice-Chair: Marjolein Thunnissen, Lund, Sweden Marjolein.Thunnissen@biochemistry.lu.se

Secretary: Gerlind Sulzenbacher, Marseille, France, Gerlind.Sulzenbacher@afmb.univ-mrs.fr