



SIG1: Macromolecular Crystallography

Reported Period: 2011-2012

Report Date: 21 May 2012

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	120
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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 120 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 Micro-crystals and Synchrotron in Life Sciences
- MS 2 Twinning, Non-crystallographic Symmetry and Space Group Determination
- MS 3 Practical Solutions to Membrane Protein Crystallography
- MS 4 Experimental Phasing in Structural Biology, Phase Improvement and Refinement
- MS 5 Crystallography, SAXS and Electron Microscopy
- MS 6 Molecular Recognition
- MS 7 Regulatory RNA
- MS 8 Macromolecular Assemblies (Viruses and Phages)
- MS 9 Cytoskeleton, Protein Trafficking and Sorting
- MS 10 Challenges in Redox-Reactions
- MS 11 Exciting new structures
- MS 12 Infection and Disease

7. Prizes sponsored/coordinated

Title : IUCr Poster Prize at ECM26, Darmstadt

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

Sponsor : IURC



Report of SIG 1 (cont.)

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

Selection Panel : Elena Boldyreva

Winning poster FA1 : MR-SAD: Phasing employing the NMR structure without model bias.
Andrea Thorn, F. Kerek, C.E.L. da Cunha, I. Uson, G.M. Sheldrick (Georg-August University, Germany; DoNatur GmbH, Germany; Inst. De Biologia Molecular de Barcelona, Spain)

Title : RCSB PDB Poster Prize at ECM26, Darmstadt

Prize : Related educational book

Sponsor : Research Collaboratory for Structural Bioinformatics Protein Data Bank

Eligibility : Best student posters related to macromolecular crystallography

Selection Panel : Wolf-Dieter Schubert, Norbert Straeter

Winning poster : Structure and Biochemistry of the APP E2-domain. Sven O. Dahms, D. Roesner, M. E. Than (Fritz Lipmann Institute, Jena, Germany)

Title : Marresearch Prize for Outstanding Young Scientist at ECM26, Darmstadt

Prize : One prize of 1000 Euro, or Two prizes of 500 Euro each if necessary

Sponsor : *Marresearch*

Eligibility : Best poster from students in the field of Crystallography and related topics; not obtained PhD yet

Selection Panel : Alessia Bacchi, Julien Haines, Wolf-Dieter Schubert

Winning poster : Mechanistic studies on ubiquitin chain formation by Triad1. Judith J. Smit, T. Hibbert, J.A. Martejijn, D.A. van der Reijden, T.K. Sixma (Netherland Cancer Institute, Amsterdam; Netherland Division of Hematology, Nijmegen, Netherlands)

8. Past Activities other than Microsymposia at ECM

Title: Erice School. Electron Crystallography – New Methods to Explore Structure and Properties of the Nano World, 2-12 June 2011, Erice, Italy

Number of Participants: over 90

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? Yes

Other Sponsors/Organizers: IURC and others

Short Description: The course intended to review structure solution using electron crystallography methods as well as novel applications.

Title: EMBO Practical Course - Exploiting Anomalous Scattering in Macromolecular Structure Determination, 6-11 June 2011, Grenoble, France

Number of Participants: 20

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: EMBO

Report of SIG 1 (cont.)

Short Description: The course aimed to impart the theoretical and practical basis for the 3-dimensional structure determination of bio-macromolecules using Anomalous Dispersion techniques (SAD & MAD) to young scientists, who intend to apply these methods in macromolecular crystallography.

Title: DGK-AK1-Workshop: Diffraction Data Collection Using Synchrotron Radiation, 7-9 July 2011, Berlin, Germany

Number of Participants: 20

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: German Society for Crystallography, DGK Working Group 1 (Biological Structures)

Short Description: The workshop included a series of basic lectures on the topic and two extended practical sessions. It was aimed at PhD students in Biological Crystallography with little or no experience in diffraction data collection at a synchrotron.

Title: 18th Summer School in Protein Crystallography, 3-9 September 2011, St Andrews, UK

Number of Participants: -

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: CCP4, BBSRC, BCA

Short Description: The course covered the theoretical and practical aspects of protein crystallography from protein expression and purification, through crystal growth to data collection on in-house and synchrotron sources, phasing methods (MAD, SAD, IR, MR) automated model building and phase extension, refinement and validation.

Title: EMBO Practical Course: Computational structural biology - from data to structure to function, 14-18 November 2011, Cambridge, UK

Number of Participants: -

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: EMBO

Short Description: This course focused on computational aspects of protein structure determination, validation and analysis. Students learned to critically examine and validate data from the Protein Data Bank and used a variety of analysis tools to identify similarities that can help identify function.

Title: CCP4 Study Week-end: Data collection and processing

Number of Participants: a few hundred

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: STFC, BBSRC, Diamond, MRC

Report of SIG 1 (cont.)

Short Description: In keeping with previous CCP4 meetings, the lectures focused on the presentation and discussion of advanced methods and techniques developed and used by the leaders in the field.

Title: 4th Winter School on soft X-rays in Macromolecular Crystallography, 6-8 February 2012, Grenoble, France

Number of Participants: 20

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: ESRF

Short Description: The Winter School aimed to bring together experts in the hardware and software required to successfully exploit anomalous signals available at long wavelengths.

Title: CECAM/CCP4 Workshop: Computational methods for macromolecular phasing and refinement, 11-17 March 2012, Zaragoza, Spain

Number of Participants: 28

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: CECAM

Short Description: The overall objective of this course is to provide an intensive practical training in all computational aspects of macromolecular structure elucidation by X-ray diffraction techniques to advanced graduate students and postdoctoral researchers.

Title: EMBO practical course on "Computational structural biology - from data to structure to function", 16-20 April 2012, Cambridge, UK

Number of Participants: -

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: EMBO

Short Description: This course focused on computational aspects of protein structure determination, validation and analysis. Students learned to critically examine and validate data from the Protein Data Bank and used a variety of analysis tools to identify similarities that can help identify function.

Title: From genes to atomic structures: an introduction to synchrotron-based structural biology, 23-26 April 2012, Trieste, Italy

Number of Participants: 49

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: IUBMB, IURC, Douglas Instruments

Report of SIG 1 (cont.)

Short Description: The school is a joint initiative between Elettra and SESAME, the new Middle East synchrotron radiation facility currently being built in Jordan, and it is directed to young scientists from all countries that are members of the United Nations, UNESCO or IAEA, with a preference for scientists coming from the Middle East. The idea is to provide the participants with a general understanding of the basic steps in structural biology (with a few hours of practicals), so as to foster further interests.

9. Future/Programmed Activities.

Various workshops and meetings are currently being organized by members of SIG1. Below is a list of events to be organized in the coming months.

Title: CECAM Collaborative Scientific Software Development meeting, 21-23 May 2012, Abingdon, UK

Number of Participants: -

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: Instruct, STFC, CCP4, WeNMR

Short Description: The workshop is intended to discuss tools aimed to help structural biologists to look beyond their own discipline, encouraging multi-disciplinary approaches including e.g. X-ray crystallography and nuclear magnetic resonance spectroscopy.

Title: CECAM Collaborative Scientific Software Development meeting, 21-23 May 2012, Abingdon, UK

Number of Participants: -

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: Instruct, STFC, CCP4, WeNMR

Short Description: The workshop intends to discuss tools aimed to help structural biologists to look beyond their own discipline, encouraging multi-disciplinary approaches including e.g. X-ray crystallography and nuclear magnetic resonance spectroscopy.

Title: Erice School. Present and Future Methods for Biomolecular Crystallography, 31 May – 10 June 2012, Erice, Italy

Number of Participants: NA

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? Yes

Other Sponsors/Organizers: IURC, IUBMB, NATO, CCP4, Bruker, ADO

Short Description: This course will help to equip the next generation of scientists with a deep understanding of the tools they need to solve challenging structural projects and an appreciation for what the future holds.



Report of SIG 1 (cont.)

Title: EMBL Advanced Course: Hybrid Structural Biology Approaches, 11 – 16 June 2012, Hamburg, Germany

Number of Participants: -

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? No

Other Sponsors/Organizers: Biostruct-X, Instruct, P3

Short Description: The course covers theoretical and experimental approaches to Small Angle X-ray Scattering (SAXS), Macromolecular Crystallography (MX) and Electron Microscopy (EM) offered at EMBL Hamburg and EMBL Heidelberg. Combined use of these structural techniques will be demonstrated and discussed.

Title: International Summer School: “Crystallography for Health and Biosciences”, 18-23 June 2012, Como, Italy

Number of Participants: 20

Level of involvement of SIG in the activity:

ECA Individual Members registered with the SIG involved in the organizing committee

ECA Individual Members registered with the SIG involved as lecturers

Sponsored by ECA? Yes

Other Sponsors/Organizers: Italian Crystallographic Association, IURC, Bruker, ICDD, Banca Popolare de Sondria, Panalytical, C.O.N.I-F.I.G.C.-C.S.I, Passing

Short Description: The purpose of the 2012 International Insubria Summer School is to explore the multiple aspects of crystallography: the world of crystallization, the more traditional and advanced experimental and computational techniques and other complementary methods, which are specifically focussed on applications in health- and bio-sciences.

10. Other matters. The last annual meeting of SIG1 took place at IUCr Congress in Madrid. The next meeting of SIG1 will be held at the ECM27 in Bergen.

11. Brief annual activity report

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: Anette Henriksen, Denmark, athx@novonordisk.com

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

Supplementary Materials.

- None