SIG1 Macromolecular Crystallography Reported Period: June 2010 – May 2011

Report Date: 31 May 2011

Reported by: Gerlind Sulzenbacher

1. Introduction.

SIG1 endeavours to unite and support the large and growing community of macromolecular crystallographers throughout Europe. This is currently a dynamic field with a continually high impact to science in general.

2. SIG web site:

http://sig1.ecanews.org/

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

SIG1 Macromolecular Crystallography

93

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 93 registered members (from http://www.xray.cz/eca/im-payment.htm), while annual meetings are normally attended by ~30 individuals. As there is no assignment of registered ECA members to SIGs, SIG1 conversely does not check that SIG1 members are individual ECA members. The current overlap is unknown. 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

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

Selection Panel : Elena Boldyreva

Winning poster FA1: MR-SAD: Phasing empolying the NMR structure without model bias. <u>Andrea Thorn</u>, 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. <u>Judith J. Smit</u>, T. Hibbert, J.A. Marteijn, 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: EMBO Practical Course on the Structural Characterization of Macromolecular

Complexes, 31 May – 5 June 2010, Grenoble

Participants: 20

Organizers: Carlo Petosa, Darren Hart, Elspeth Gordon, Guy Schoehn, Winfried

Weissenhorn

Sponsors: EMBO

Description: A course primarily intended for Ph.D. students and postdocs engaged in

challenging structural projects involving macromolecular complexes

Title: Erice School. Structure and Function from Macromolecular Crystallography:

Organisation in Space and Time, 3-13 June 2010, Erice, Italy

SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing

committee and giving lectures

ECA sponsored: YES

Sponsors: IUCr, IUBMB, IUSF, Rigaku, Oxford Diffraction, Astra Zeneca, Bruker, Dougla

Instruments

Organizers: Tom Blundell, Maria Armenia Carrondo, John Irvin, Lodovico Riva, Paola

Spadon

Description: The objective of this meeting is to introduce students to the use of advanced

techniques for the study of structures of macromolecular assemblies involving

protein, DNA, RNA and polysaccharide.

Title: EMBO Practical Course. Protein Expression, Purification and Crystallisation,

23-31 August 2010, EMBL Hamburg, Germany

ECA sponsored: No **Sponsors:** EMBO

Organizers: Rob Meijers, Jochen Mueller-Dieckmann, Young Hwa-Song

Description: The course will cover over-expression of proteins in prokaryotic and eukaryotic

systems, protein purification and characterisation, crystallization techniques and

determination of crystal quality.

Title: 8th International NCCR Symposium on New Trends in Structural Biology, 2-3

September 2010, Zuerich, Switzerland

ECA sponsored: NO

Organizers: Patrick Sticher Moser

Description: This symposium series provides a yearly update on current structural biology

and newest developments in the field.

Title: EMBO Practical Course 'Computational aspects of protein structure

determination and analysis: from data to structure to function', 6-10 September

2010, EMBL-EBI Cambridge, UK

SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing

committee

ECA sponsored: NO **Sponsors:** EMBO

Organizers: Gerard Kleywegt, Victor Lamzin, Christine Orengo, Gert Vriend, James Watson,

Rosemary Wilson

Description: The goal of the course is to provide insight into the protein structure

determination process, assessment of structure quality and analysis of protein

structure data with a view to predicting protein function.

Title: 13th International Conference on the Crystallization of Biological

macromolecules, 12-16 September 2010, Dublin, Ireland

SIG1 level: ECA Individual Members registered with the SIG1 involved in lectures

ECA sponsored: NO

Sponsors: IURC + others **Organizers:** Martin Caffrey

Description: The meeting of choice to learn about the latest research and developments in

biomacromolecular crystallogenesis for structure-function-rational design applications. At ICCBM13 leading academic and pharmaceutical scientists will report on challenging systems to include macromolecular complexes and membrane proteins with an emphasis on novel practical as well as mechanistic aspects of crystallogenesis. To cater to the needs of the individual wanting to learn how to grow crystals or to acquire new crystallization skills, the Conference is preceded by a Workshop (9-12 September) devoted to hands-on instruction on select aspects of macromolecule production and crystal growth.

Title: BioCrys2010 Fundamentals of Modern Methods in Biocrystallography - 'What

you always wanted to know about crystallography but never dared to ask', 9-16

October 2010, Oeiras, Portugal

Participants: 36

SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing

committee and involved in lectures

ECA sponsored: NO Sponsors: FEBS, IUCr

Organizers: Maria Arménia Carrondo, Thomas Schneider

Description: The fifth BioCrys course focuses on Macromolecular Crystallography, by

developing the fundamental concepts of crystallography and illustrate these by

tutorials and practical sessions.

Title: Advances in Protein Crystallography, 9-10 November 2010, Florence, Italy.

SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing

committee

ECA Individual Members registered with the SIG1 involved as lecturers

ECA sponsored: NO

Description: Protein Chemistry and Crystallization, New Laboratory Instrumentation and

Techniques, Advances in Diffraction Techniques and Crystallographic

Computing, New Drug Target Structures and their Analysis

Title: CCP4 Study Week-end: "Model Building & Refinement & Validation", 5-7

January 2011, Warwick, UK

SIG1 level: ECA Individual Members registered with the SIG1 involved as lecturers

ECA sponsored: NO

Organizers: Roberto Steiner, Bernhard Rupp

Description: Meeting with lectures focused on the presentation and discussion of advanced

methods and techniques developed and used by the leaders in the field. The meeting offers a chance to meet the CCP4 staff, who will be there in force to

demonstrate the latest software and to answer questions.

Title: Intensive 2-day School in Biological and Chemical Crystallography, 11-12

January 2011, Manchester, UK

SIG1 level: ECA Individual Members registered with the SIG1 involved organization and

lecturing

ECA sponsored: NO **Sponsors:** IURC

Organizers: John Helliwell, Christine Taylor

Description: CPD (continuing professional development) training opportunity for Research

and technical staff in R&D laboratories, University academics, Postdoctoral and

postgraduate researchers, Industrial R&D Managers, Biochemical,

Biotechnology and Healthcare professionals, IT professionals, School teachers.

Title: OPPF-MPL High-throughput Protein Production and Crystallization, 30 March-7

April 2011, Didcot, UK

Participants: 12 ECA sponsored: NO

Sponsors: OPPF-UK, MPL

Organizers: Ray Owens, Isabel Moraes

Description: The aim of this course will be to review the state-of-the-art in HTP structural

biology with an emphasis on methods to study complex and 'difficult' targets including membrane proteins. This workshop brings together renowned scientists expert in the production, crystallisation and structure determination

of membrane proteins.

Title: 2nd Advanced Protein Characterisation and Crystallisation Course, 2-6 May,

2011, Helsinki, Finland

ECA sponsored: NO

Organizers: Tommi Kajander

Title: International School on Biological Crystallization (ISBC 2011), 22-26 May 2011,

Granada, Spain

Participants: 40

SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing

committee and involved in lecturers

ECA sponsored: NO

Sponsors: IUCr and others

Organizers: Juan Manuel Garcia-Ruiz, José Antonio Gavira, Alfonso García Caballero, Luis

Antonio González Ramírez, Estela Pineda Molina, Jose Manuel Delgado Lopez

Description: A school oriented to postgraduate/postdoctoral students and research scientists

from industry and academy, who are interested in the fundamental knowledge

of crystallization.

9. Future/Programmed Activities.

Various workshops and meetings are currently being organized by members of SIG1.

Title: EMBO Practical Course: Exploiting Anomalous Scattering in Macromolecular

Structure Determination, 6-10 June 2011, Grenoble, France

ECA sponsored: No **Sponsors:** EMBO

Organizers: Daniele de Sanctis, Christoph Mueller-Dieckmann, Gordon Leonard, Didier

Nurizzo, Claudine Romero, Hassan Belrhali, Andrew McCarthy

Description: The course aims 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: Advances in Protein Crystallography 2011, 30 June- 1 July, Hamburg, Germany

Title: EMBO Practical Course on High Throughput methods for protein production

and crystallization, 4-14 July 2011, Marseille, France

SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing

committee and involved as lecturers

ECA sponsored: No **Sponsors:** EMBO

Organizers: Yves Bourne, Bruno Coutard, Gerlind Sulzenbacher, Florence Vincent, Renaud

Vincentelli

Description: The course is intended for PhD students and young researchers using

highthroughput methods for expression and crystallization of soluble proteins. The goal is to provide participants with the current knowledge in the use of the

most innovative methods in the field.

Title: Diffraction Data Collection Using Synchrotron Radiation, 7-9 July 2011,

Helmholtz Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany

Participants: 20

SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing

committee and involved as lectures

ECA sponsored: NO

Sponsors: German Society for Crystallography (DGK)

Organizers: German Society for Crystallography (DGK) Working Group 1 (Biological

Structures) in cooperation with Dr. Uwe Mueller (BESSY, Berlin).

Description: Workshop aimed at PhD students in Biological Crystallography with little or no

experience in diffraction data collection at a synchrotron. The practical session took place at the MX beamlines located at the electron storage ring BESSY II.

Title: 9th International NCCR Symposium on New Trends in Structural Biology, 1-2

September 2011, Zuerich, Switzerland

ECA sponsored: NO

Organizers: Patrick Sticher Moser

Description: This symposium series provides a yearly update on current structural biology

and newest developments in the field.

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

Andrews, UK

Organizers: Garry Taylor, Jim Naismith

10. Other matters.

The annual meeting of SIG1 took place at the ECM26 in Darmstadt, Germany. The next meeting of SIG1 will be held at IUCr Congress in Madrid

11. Brief annual activity report

The main activity of SIG1 involves the organization of the microsymposia 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 of SIG officers:

Chair: Keith Wilson, York, United Kingdom, keith@ysbl.york.ac.uk **Vice-Chair:** Anette Henriksen, Valby, Denmark, anette@crc.dk

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

mrs.fr

Supplementary Materials.

- None