

SIG1 Macromolecular Crystallography
Reported Period: January 2009 – May 2010
Report Date: 31 May 2010
Reported by: Gerlind Sulzenbacher

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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:

Under construction

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

SIG1 Macromolecular Crystallography 77

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 77 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 Large Macromolecular Complexes
- MS 2 50 Years of Globins
- MS 3 Novel Enzyme Mechanisms
- MS 4 Molecular Transport and Recognition
- MS 5 Structural Basis of Pathogenesis
- MS 7 Molecular Recognition and Drug Design
- MS 8 Membrane Proteins: Frontiers and Challenges
- MS 9 Practical Protein Production, Purification and Crystallization
- MS 10 Computational Methods in Macromolecular Crystallography
- MS 11 Complementary Biophysical Techniques
- MS 12 High Throughput and Model Validation in Macromolecular Crystallography
- MS 13 NMR, Crystallography and Macromolecular Structure
- MS 14 Very High Resolution Protein Structures

7. Prizes sponsored/coordinated

Title : IUCr Poster Prize at ECM25, Istanbul.

Prize : Two 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 & FA3

Selection Panel : Paola Gilli, Janusz Lipkowski, Grzegorz Bujac, Mathias Bochtler

Winning poster : The Structure of DapD from Mycobacterium tuberculosis . Linda Schulda, Simone Weyanda, Georgia Kefalaa, Manfred S. Weiss (*EMBL Hamburg Outstation, c/o DESY*)

Title : RCSB PDB Poster Prize at ECM25, Istanbul

Prize : Related educational book

Sponsor : Research Collaboratory for Structural Bioinformatics Protein Data Bank

Eligibility : Best student posters related to macromolecular crystallography

Selection Panel : Elspeth Garman, Joel Sussman

Winning poster : Crystallization of bifunctional catalase-phenol oxidase (CATPO) from *Scytalidium thermophilum* . Yonca Yuzugullua, Chi Trinha, Arwen R. Pearson, Mark A. Smitha, Simon Phillipsa, Ufuk Bakira, Michael J. McPhersona, Zumurut B. Ogela (*Food Engineering Department, University of Leeds, UK*)

Title : Marresearch Prize for Outstanding Young Scientist at ECM25, Istanbul

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 : Fernando Lahoz, Gerlind Sulzenbacher, Olga Yakubovich

Winning poster : Sticky Triangles for Experimental Phasing. Tobias Becka, Tim Gruenea, George M. Sheldrick (*Department of Structural Chemistry, Georg-August-Universität Göttingen, Germany*)

8. Past Activities other than Microsymposia at ECM

Title: CCP4 Study Weekend: "Experimental Phasing and Radiation Damage", Nottingham, UK, 3-5 January 2009

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

Sponsors: BBSRC, Science & Technology Facility Council

Organizers: Clemens Vonrhein, Elspeth Garman, Arwen Pearson

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: French Structural Biology Day, Lyon-Gerland, France, January 15th, 2009

Participants: 50

ECA sponsored: NO

Organizers: Eva Pebay-Peyroula, Yves Bourne, Dino Moras, Stephen Cusak, Félix Rey

Description: The purpose of the meeting is to take stock of the current state of structural biology in France in terms of ongoing projects, positioning within the wider European context, and long-term vision.

Title: MX School "Getting the most from the ESRF MX beamlines", Grenoble, France, 2-6 February 2009

Participants: 20

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

ECA sponsored: NO

Sponsors: ESRF

Organizers: Gordon Leonard, Didier Nurizzo

Description: The "Getting the most from the ESRF MX beamlines" school is aimed at *younger scientists* and designed to (a) introduce the art of collecting good diffraction data at synchrotron-based MX facilities, (b) familiarize the participants with the tools available at the beam-line to allow pre- and post-data decisions to be taken and (c) present the various ancillary techniques and equipment accessible at the ESRF's Structural Biology beamlines.

Title: Winter School on Soft X-rays in Macromolecular Crystallography, BESSY-II, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany, 18-20 February 2009

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

Organizers: Uwe Mueller, Manfred Weiss, Kristina Djinovic Carugo

Description: The third Winter School on Soft X-rays in Macromolecular Crystallography will bring together experts from different fields, which are key-players in the developments and further utilization of soft X-ray applications in structural biology with the users of this modern methodology.

Title: INSTRUCT Italian Users' meeting, Florence, Italy, 24 March 2009

Participants: 60

ECA sponsored: NO

Organizers: Ivano Bertini, Kathleen McGreevy

Description: Users' Meeting directed at the Italian Structural Biology community and those interested in the exploitation of the results of Integrated Structural Biology.

Title: International School on Biological Crystallization (ISBC 2009), Granada, Spain, 18-22 May 2009

Participants: 40

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

Sponsors: IUCr, University of Grenada, GE3C, Bruker, Hampton Research, IZASA Werfen Group, Triana Sci & Tech, La Factoria, CSIC, UIMP, Molecular Dimensions, JenaBioscience, OptiCryst, Sigma-Aldrich, Aston University, e-MeP Lab.

Organizers: Juan Manuel Garcia-Ruiz, José Antonio Gavira, Jaime Gomez-Morales, Fermin Otálora, Luis Antonio González Ramírez, Alfonso García Caballero.

Description: A school oriented to postgraduate/postdoctoral students and research scientists from industry and academy, who are interested in the fundamental knowledge of crystallization.

Title: Membrane Protein Production, Crystallization and Crystallography, Diamond Light Source, Didcot, UK, 2-4 June 2009

Participants: 30

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

ECA sponsored: NO

Sponsors: E-MEP-Lab framework 6 European Union training grant

Organizers: Liz Carpenter, Konstantinos Beis, Alexander Cameron in collaboration with The Membrane Protein Laboratory and Diamond Light Source Ltd.
Description: This workshop brings together renowned scientists expert in the production, crystallisation and structure determination of membrane proteins.

Title: EMBO / MAX-INF2 2009 Practical Course on Structure Determination in Macromolecular Structure, ESRF-EMBL, Grenoble, France, 15 - 19 June 2009
Participants: 20
SIG1 level: ECA Individual Members registered with the SIG1 involved as lecturers
ECA sponsored: NO
Sponsors: EMBO, MAX-INF2, ESRF, EMBL
Organizers: Christoph Müller-Dieckmann, Gordon Leonard, Didier Nurizzo, Matthew Bowler, Claudine Roméro, Andrew McCarthy
Description: This practical course addresses young scientists who intend to apply single and multiple wavelength anomalous scattering (SAD & MAD) methods in macromolecular structure determination.

Title: EMBO Practical Course. High throughput methods for protein production and crystallization, Oxford, UK, 17-25 June 2009
Participants: 20
ECA sponsored: NO
Sponsors: EMBO
Organizers: Ray Owens, Dave Stuart, Ian Jones, Karl Harlos, Susan Daenke
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.

Title: Protein Crystallography Europe Conference, Amsterdam, The Netherlands, 19-20 June, 2009
SIG1 level: ECA Individual Members registered with the SIG1 involved as lecturers
ECA sponsored: NO

Title: Practical Workshop on Characterization of Protein Complexes in Structural Biology, EMBL-Hamburg, Germany, 30 June - 3 July 2009.
SIG1 level: ECA Individual Members registered with the SIG1 involved as lecturers
ECA sponsored: NO
Sponsors: EU funded projects SPINE2-complexes, 3D Repertoire, PENELOPE and Teach-SG
Organizers: Jochen Mueller-Dieckmann, Maxim Petoukhov, Dmitri Svergun, Vivian Pogenberg, Young-Hwa Song, Matthias Wilmanns, Rosemary Wilson, Michela Bertero
Description: Workshop aimed at advanced graduate students and postdoctoral fellows interested in expanding their knowledge of state-of-the-art biophysical and biochemical characterization methods of protein complexes. A workshop including hands-on sessions and lectures by world-leading experts from relevant fields. Topics covered: FRET, BIFC, SAXS, ITC, high-throughput crystallization and mass spectrometry.

Title: Diffraction Data Collection Using Synchrotron Radiation, Helmholtz Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany, 13-15 August, 2009
Participants: 20
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
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: 7th International NCCR Symposium on New Trends in Structural Biology, Zuerich, Switzerland, 7-9 September 2009

Participants: 340

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: BioCrys Course: Macromolecular Crystallography, Oeiras, Portugal, 4-11 October 2009

Participants: 36

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

Sponsors: MAX-INF2, SPINEComplexes, Teach-SG

Organizers: Maria Arménia Carrondo, Thomas Schneider

Description: The fourth BioCrys course focuses on Macromolecular Crystallography, by developing the fundamental concepts of crystallography and illustrate these by tutorials and practical sessions.

Title: EMBO Practical Course. The combination of electron microscopy and X-ray crystallography for the structure determination of large biological complexes, Grenoble, France, 18 - 24 October, 2009

Participants: 20

ECA sponsored: NO

Sponsors: EMBO

Organizers: Jorge Navaza, Laurence Serre, Leandro F. Estrozi, Jean Lepault, Felix Rey

Description: The course aims to train junior investigators in both fields (electron microscopy and X-ray crystallography) to carry out their combined use in their home institutes. The participants will be introduced to underlying theoretical aspects of the used methods but emphasis will be given to the practical work and problem solving.

Title: Practical Course on Training in Methods for Macromolecular Crystallography M2M-2009: From Measurement to Model, EMBL Hamburg Outstation, Germany, 21-28 October, 2009

Participants: 20

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

Sponsors: European Macromolecular Crystallography Infrastructure network (MAXINF2), EC Contract No 505977

Organizers: Victor Lamzin, Santosh Panjikar, Thomas Schneider, Paul Tucker, Manfred Weiss

Description: The M2M course covers the essential steps in determining biomolecular structures. The M2M-2009 course includes practicals at synchrotron beamlines for macromolecular crystallography, computational tutorials and lectures on the use of synchrotron radiation and beamline equipment, sample handling and carrying out an experiment.

Title: CCP4 Study Weekend: From Crystal to Structure with CCP4, Nottingham, UK, 6-8 January 2010
SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing committee
ECA sponsored: NO
Sponsors: BBSRC, MRC, Science & Technology Facility Council, Diamond
Organizers: Keith Wilson, Kevin Cowtan, Paul Emsley
Description: Meeting with lectures focused on the presentation and discussion of advanced methods and techniques developed and used by the leaders in the field. A chance to meet the CCP4 staff who will be there in force to demonstrate the latest software and to answer questions.

Title: Correlative Microscopy Workshop, Oxford, UK, 13-14 January 2010
SIG1 level: ECA Individual Members registered with the SIG1 involved as lecturers
ECA sponsored: NO
Sponsors: INSTRUCT FP7-211252
Description: Workshop aimed at developing an understanding of the major scientific problems which could be addressed by a combination of microscopy and imaging based modalities in conjunction with other structural based techniques such as crystallography.

Title: MX School "Getting the most from the ESRF MX beamlines", Grenoble, France, 8-12 February 2010
Participants: 20
SIG1 level: ECA Individual Members registered with the SIG1 involved as lecturers
ECA sponsored: NO
Sponsors: ESRF
Organizers: Gordon Leonard, Daniele de Sanctis
Description: The school is aimed at *younger scientists* and designed to (a) introduce the art of collecting good diffraction data at synchrotron-based MX facilities, (b) familiarize the participants with the tools available at the beam-line to allow pre- and post-data decisions to be taken and (c) present the various ancillary techniques and equipment accessible at the ESRF's Structural Biology beamlines.

Title: From Crystals to Structures: CCP4 Seminar and Workshop, New Delhi, India, 15-19 February 2010
SIG1 level: ECA Individual Members registered with the SIG1 involved in the organizing committee
ECA sponsored: NO
Sponsors: CCP4
Organizers: CCP4
Description: The course is intended mainly for graduate students and postdoctoral researchers in the area of structural biology from all across the globe. The purpose of the school is to address specific problems that the applicants face while processing diffraction data and while solving and refining novel structures.

Title: Practical Workshop on the use of Longer Wavelengths in Structural Biology, Grenoble, France, 18-19 February 2010
Participants: 6
SIG1 level: ECA Individual Members registered with the SIG1 involved as lecturers
ECA sponsored: NO
Sponsors: ESRF
Organizers: Claudine Roméro, Daniele de Sanctis, Gordon Leonard, Christoph Müller-Dieckmann
Description: A practical workshop on the use of longer wavelengths in Structural Biology

Title: EMBO Conference Series. Catalytic mechanisms by biological systems: at the Interface between chemistry and biology, EMBL-Hamburg, Germany, 5-7 May 2010

Participants: 120

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

ECA sponsored: NO

Sponsors: EMBO

Organizers: Andre Juffer, Maja Koeln, Anne-Marie Lambeir, Victor Lamzin, Andrea Mattevi, Andrea Schmidt, Reinhard Sterner, Rik Wierenga

Description: The conference is aimed at bringing together experts working at the interface of this multidisciplinary research field to facilitate stimulating discussions on this fascinating topic, which is also of key importance for the development of biotech related applications.

Title: 3rd International Symposium on Diffraction Structural Biology (ISDSB2010), Paris, France, 25-28 Mai 2010

Participants: 200

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

ECA sponsored: YES

Sponsors: University-Industry Cooperative Research Committee (#169) of Japan Society for the Promotion of Science (JSPS), ECA, IUCr

Organizers: Roger Fourme, John R Helliwell, Jack Johnson, Noriyoshi Sakabe, Noritake Yasuoka

Description: The historical concept of the ISDSB Symposia is to bring together researchers using diffraction and crystallography, and more generally interactions of X-rays, electrons and neutrons with matter in the study of structural biology and, secondly, within this domain to facilitate the interaction between academic and industrial researchers.

9. Future/Programmed Activities.

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

Title: EMBO Practical Course on the Structural Characterization of Macromolecular Complexes, Grenoble, France, 31 May – 5 June 2010

ECA sponsored: No

Sponsors: EMBO

Organizers: Espeth Gordon, Darren Hart, Carlo Petosa, , Guy Schoehn, Winfrid Weissenhorn

Description: This EMBO practical course aims to teach the strategic use of various biochemical and biophysical techniques to facilitate structural studies of macromolecular complexes.

Title: Erice School. Structure and Function from Macromolecular Crystallography: Organisation in Space and Time, Erice, Italy, 3-13 June 2010

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

Sponsors: IUCr, IUBMB, IUSF, Rigaku, Oxford Diffraction, Astra Zeneca, Bruker, Dougl 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, EMBL Hamburg, Germany, 23-31 August 2010

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: EMBO Practical Course 'Computational aspects of protein structure determination and analysis: from data to structure to function', EMBL-EBI Cambridge, UK, 6-10 September 2010

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: BioCrys2010 Fundamentals of Modern Methods in Biocrystallography - 'What you always wanted to know about crystallography but never dared to ask', Oeiras, Portugal, 9-16 October 2010

Participants: 36

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

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.

10. Other matters.

The annual meeting of SIG1 took place at the ECM25 in Istanbul, Turkey. Because the previous Vice-Chair and Secretary of SIG1, Matthias Bochtler and Wolf-Dieter Schubert, respectively, were unable to continue in their positions due to other commitments, it was necessary to elect new members to these positions. This was carried out in an open meeting of SIG1 at the Istanbul ECM25. Anette Henriksen was elected Vice-Chair and Gerlind Sulzenbacher was elected Secretary. The next meeting of SIG1 will be at the ECM26 2010 in Darmstadt, Germany.

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

The main activity of SIG1 involves the organization of the microsymbosia 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, Valby, Denmark (anette@crc.dk)

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

Supplementary Materials.

- None

