

**SIG: 1 Macromolecular Crystallography**

**Reported Period: 2008-2009**

**Report Date: 31 May 2009**

**Reported by: Wolf-Dieter Schubert**

**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. Past Activities.**

The main function of SIG1 at present is to represent the interests of the structural biology community in Europe in general and in particular in the run-up to the annual meetings of the ECA.

A selection of workshops, seminars and courses organized by the European structural biology community include:

**Title:** Structural and Molecular Biology of Host-Pathogen Interactions, Grenoble, France, 5-7 February, 2008.

**Participants:** 25

**Organizers:** Laurent Terradot, Myriam Dhez, Andrea Dessen, Dominique Housset, Daniel Panne, Winfried Weissenhorn

**Sponsors:** ESRF, EMBL

**Description:** Topics of the workshop include bacterial adhesion to the host cell, bacterial secretion of toxins, virus replication and host cell factors, subversion of the immune system, host-cell response.

**Title:** CCP4 Workshop on Computational Crystallography – Bangalore, Indian Institute of Science, Bangalore, India, 18 – 22 February 2008.

**Participants:** 100

**Organizers:** Martyn Winn, Paul Emsley, Eleanor Dodson

**Sponsors:** BBSRC

**Description:** A workshop to introduce and support the use of crystallographic software and skills in India. The workshop was attended by graduate students from all 33 structural biology groups in India.

**Title:** South West Structural Biology Consortium (SWSBC 2008), 31 March - 1 April 2008

**Participants:** 100

**Organizers:**

**Sponsors:** CCP4

**Description:** The conference circles around universities in the South West UK with an interest in structural biology. The programme consisted of an invited outside lecture, short oral presentations from academics/postdocs and PhD students from the Universities in the South West of the UK and poster sessions. Participants represented leading edge research and business opportunities in the area of structural biology.

**Title:** 6th TID Workshop: Biocrystallography with Synchrotron Radiation, Center for Biocrystallographic Research (BIOXHIT TID Centre), Poznan, Poland, 6-9 April 2008.

**Participants:** 21

**Organizers:** Mariusz Jaskolski

**Sponsors:** BIOXHIT

**Description:** This workshop for pre-doctoral students and post-doctoral fellows from 7 European countries pioneered remote data collection at the ESRF in the field of bio-crystallography.

**Title:** Synchrotrons and Lasers for Structural Systems Biology, Symposium EMBL Hamburg, Germany, 16 April 2008.

**Participants:** 140

**Organizers:** Gerard Bricogne, Kim Henrick, Victor Lamzin, Sine Larsen, Sean McSweeney, Colin Nave, Anastassis Perrakis, Manfred Weiss.

**Sponsors:** BIOXHIT

**Description:** International experts in the field of the use of synchrotron radiation in biological research presented their view of the future of Structural Biology once the new X-ray sources become available.

**Title:** 4th annual meeting of the BIOXHIT Integrated Project (Biocrystallography (X) on a Highly Integrated Technology Platform for European Structural Genomics), EMBL Hamburg, Germany, 17 - 18 April 2008.

**Participants:** 140

**Organizers:** Gerard Bricogne, Kim Henrick, Victor Lamzin, Sine Larsen, Sean McSweeney, Colin Nave, Anastassis Perrakis, Manfred Weiss.

**Sponsors:** BIOXHIT

**Description:** The scientific highlights of the BIOXHIT project including those from the four BIOXHIT TID centres and representatives of the user community were presented. The meeting was accompanied by poster presentations from the project partners and external attendees. The topics covered crystallisation technology, synchrotron beamlines, beamline end-stations and data collection, data processing and structure determination, databases and networking, training, implementation and dissemination.

**Title:** Workshop & International School on Macromolecular Crystallization, Cancun, Mexico, 2 - 5 May 2008.

**Participants:** 30

**Organizers:** Naomi Chayen, Richard Giegé, Alexander McPherson, Juan Manuel García-Ruiz, Sheng-Xiang Lin, Martin Caffrey

**Sponsors:** IUCr, UNAM, IOBCr, CTIC, IQ-UNAM, CONACYT

**Description:** Theory and Practical Aspects of Protein Crystallization

**Title:** ICCBM12, the 12th International Conference on the Crystallization of Biological Macromolecules, Cancun, Mexico, 6 - 9 May 2008.

**Participants:** 300

**Organizers:** Naomi Chayen, Richard Giegé, Alexander McPherson, Juan Manuel García-Ruiz, Sheng-Xiang Lin, Martin Caffrey

**Sponsors:** IUCr, UNAM, IOBCr, CTIC, IQ-UNAM, CONACYT

**Description:** Much progress has been made in macromolecular crystallization research. The demand for crystals for the study of biological structures nevertheless continues to increase. Genomic and Proteomic projects have begun the transition into a structural proteomics phase, supported by various approaches, including high throughput, microfluidics for protein crystal growth (PCG). Clearly, structural genomics has made great strides in increasing our understanding of biological structure, but the overall success rate of PCG, even in genomic projects, remains distressingly and unacceptably low.

**Title:** Maxinf2 Workshop on New Algorithms in Macromolecular Crystallography and Electron Microscopy, Leiden, The Netherlands, 13 - 17 May 2008.

**Participants:** 50

**Organizers:** Navraj Pannu, Raimond Ravelli, Jan-Pieter Abrahams

**Sponsors:** Maxinf2, the Lorentz Centre, Cyttron, Fei and Bruker

**Description:** The workshop brought together scientists active in computational methods development in X-ray crystallography and those working in electron microscopy with an aim to accelerate the development of future algorithms and to allow the optimal use of the information obtainable from both techniques.

**Title:** Virtual Discovery and Advances in Protein Crystallography, Amsterdam, The Netherlands, 19-20 June 2008.

**Participants:** 200

**Organizers:** Protein Crystallography.com and *inter alia* Naomi Chayen,

**Sponsors:** Waters, TTP Labtech, Bentham Scientific, Protein Crystallography.com, biocompare, CombiChem, Future Pharmaceuticals, GenomicsProteomics.com, HTS Screening.net, Labhoo.com, Scientific Computing World.

**Description:** Topics: Protein Chemistry and Crystallization, New Laboratory Instrumentation and Techniques, Advances in Diffraction Techniques and Crystallographic Computing, New Drug Target Structures and their Analysis.

**Title:** BIOXHIT course "S-SAD diffraction data phasing of macromolecule single crystals from home and synchrotron X-ray sources, ITQB, Oeiras, Portugal, 19 - 21 June 2008

**Participants:** 30

**Organizers:** Pedro Matias, Daniele de Sanctis

**Sponsors:** BIOXHIT

**Description:** A course highlighting the use of the weak anomalous scattering from sulfur atoms in protein crystals to derive phase information using highly redundant and accurate data measured from a rotating anode or a synchrotron source.

**Title:** BIOXHIT-Course "From Crystals to Structures", IMBB-FORTH, Heraklion, Greece, 23 - 25 June 2008.

**Participants:** 20

**Organizers:** Evangelia G. Kapetaniou, Michael Kokkinidis, Spyros Zographos, Nikos G. Oikonomakos, Renate Gessmann, Kyriacos Petratos

**Sponsors:** BIOXHIT

**Description:** This workshop was addressed primarily to pre-doctoral students and young post-doctoral fellows in the field of bio-crystallography residing in Greece and the wider Balkan region.

**Title:** 11th Heart of Europe Bio-Crystallography Meeting, "HEC-11", Greifswald, Germany, 25 - 27 September 2008.

**Participants:** 160

**Organizers:** Winfried Hinrichs, Daniela Dalm, Gottfried Palm

**Sponsors:** Rigaku, JenaBioscience, Dunn, HKL Research Inc., greinier bio-one, Sparkasse Vorpommern, GBM, Incoatec, IUCr, Bruker, IBA, GE Healthcare, Oxford diffraction, GE, Zinsser Analytic

**Description:** The scientific sessions of the three-day conference will consist of an invited lecture from an eminent scientist and lectures from young research scholars. It is the important task of HEC meetings to encourage young researchers to present and share their achievements and difficulties. This is the major difference to common scientific meetings.

**Title:** FEBS Advanced Course "Advanced methods in protein crystallization", Academic and University Centre, Nove Hrad, Czech Republic, 3-10 October 2008.

**Participants:** 30

**Organizers:** Ivana Kutá Smatanová, Pavlína Řezáčová, Rolf Hilgenfeld

**Sponsors:** Hampton Research, Triana Sci&Tech, Olympus, Quiagen, Molecular Dimensions, Limited, Emerald Biosystems, Douglas Instruments, Wyatt Technology, BioConsult, Bruker AXS, Czech and Slovak Crystallographic Association, Eppendorf, FEBS, JenaBioScience

**Description:** The course is intended for undergraduate (5th year) and postgraduate students and postdocs with an interest in macromolecular crystallization.

**Title:** BIOCRYST 2008 Fundamentals of Modern Methods in Biocrystallography, Instituto de Tecnologia Química e Biológica, Oeiras, Portugal, 4 - 11 October 2008.

**Participants:** 36

**Organizers:** Maria Arménia Carrondo, Thomas Schneider

**Sponsors:** MAX-INF2, SPINEComplexes, Teach-SG

**Description:** The topics of this course spanned fundamentals such as symmetry, point groups and crystal systems, basic diffraction physics, reciprocal space and the Ewalds sphere, radiation damage, data processing, structure factors, Patterson function to modern methodologies including molecular replacement, SAD, MAD, MIR and maximum likelihood phasing, density modification, refinement, model building, twinning and structure validation.

**Title:** EMBO World Lecture Course: Recent Developments in Macromolecular Crystallography, National Chemical Laboratory (NCL), Pune, India, 9 - 14 November 2008.

**Participants:** 200

**Organizers:** Manfred S. Weiss, C.G. Suresh, Paul Tucker, Santosh Panjikar, Sanjay Nene.

**Sponsors:** EMBL, National Chemical Laboratory (NCL, India), CSIR (India), Hampton Research, Rigaku, Incoatec, JenaBioscience, Oxford Diffraction, Bruker, Douglas Instruments.

**Description:** This course consisted of lectures describing recent methodological developments in the field from crystallization, to diffraction data collection, structure determination and function prediction from structure. Further lectures will be on recent achievements in biology using X-ray diffraction techniques.

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

**Participants:** 50

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

**Sponsors:**

**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:** International School on Biological Crystallization. Granada, Spain, May 2009

**Participants:** 40

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

**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.

**Description:** This International School focused on the fundamentals of crystallisation from solutions and its applications to the field of the crystallisation of biological materials. The School will provide five days of lectures and practical demonstrations related to the crystallisation of biological macromolecules, biominerals and biomimetic materials, with one full day devoted to case studies on the crystallisation of membrane proteins and large macromolecular complexes.

### 3. Future/Programmed Activities.

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

### 4. Other matters:

Because of the Meeting of the IUCr in Japan in 2008, no separate ECM meeting was convened in 2008. As such there was also no annual meeting of SIG1.

### 5. Five year 'overview', brief activity report (2005-2009)

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 increasing 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.

### 6. Estimated number of active members:

SIG1 currently has 65 registered members, 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.

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

**SIG1 Committee:**

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

**Vice-Chair:** Matthias Bochtler, Warsaw, Poland (mbochtler@iimcb.gov.pl)/ Cardiff, UK

**Secretary:** Wolf-Dieter Schubert, Braunschweig, Germany (wds@helmholtz-hzi.de)

**Further members:**

Mariusz Jaskolski, Posnan, Poland (mariuszj@amu.edu.pl)

Victor Lamzin, Hamburg, Germany (victor@embl-hamburg.de)

Anette Hendriksen, Valby, Denmark (anette@crc.dk)

Naomi Chayen, London, United Kingdom (n.chayen@imperial.ac.uk)

Manfred Weiss, Hamburg, Germany (msweiss@embl-hamburg.de)

Anders Liljas, Lund, Sweden (Anders.Liljas@mbfys.lu.se)

Frank von Delft, Oxford, United Kingdom (frank.vondelft@sgc.ox.ac.uk)

Maria Arménia Carrondo, Oeiras, Portugal (carrondo@itqb.unl.pt)

**Supplementary Materials.**

None