

SIG1: Macromolecular Crystallography

Reported Period: 2017-2018

Report Date: 22 August 2018

Reported by: Marjolein Thunnissen, Jan Dohnalek, Ronan Keegan

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://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	318
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4. Existence of a SIG mailing list : Yes

Address of the mailing list: <https://groups.google.com/forum/#!forum/sig1eca>

Number of members in the SIG mailing list : 31

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

SIG1 currently has 318 registered members (from <http://www.xray.cz/eca/eca-sig.asp?id=SIG1>), while meetings are normally attended by ~30-50 individuals. Several dozens of researchers are involved in SIG1 activities, especially in the organization of courses and workshops.

6. List of MS organized by the SIG at the last ECM (ECM30)

MS1 - SAXS in structural biology

MS2 - Development of new types of sample preparation (both XFEL & synchrotrons)

MS3 - Data collection and processing software (XFELS & synchrotrons)

MS4 - New developments in phasing and refinement

MS5 - Structural information in drug design

MS6 - Molecular machines and big complexes

MS7 - Protein & glycobiochemistry structure determination

MS8 - Membranes and membrane interacting proteins

MS9 - Enzyme reactions and dynamics in crystals

MS10 - H-bonding & weak interactions in crystals: neutrons and X-rays

MS11 - Hybrid approaches and validation (X-ray and electron microscopy)

MS12 - Biophysical characterization and crystallization

MS13 - Hot structures in biology

7. Prizes sponsored/coordinated

N/A

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. ECM sponsored activities include the 20th Heart of Europe Bio-Crystallography Meeting at Wojanów Palace, Poland September 28th to 30th 2017, the 2018 Diamond/CCP4 Data collection and Structure Solution Workshop from November 30th to December 7th 2017, and the Hot topics in contemporary crystallography 2018 (HTCC3), organized by the Croatian Association of Crystallographers, to be held in Poreč, Croatia, from September 22-27, 2018.

9. Future/Programmed Activities.

Currently SIG1 is actively involved in the planning of the microsymposia for the forthcoming ECM32 meeting in Vienna, Austria. Marjolein Thunnissen is the main contact from SIG1 for this activity. A list of microsymposia has been proposed that balances the different interests of SIG1 regarding science as well as methods and instrument development.

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 as well as iNEXT (<http://www.inext-eu.org/>).

10. Other matters. The next annual meeting of SIG1 will take place at ECM31 in Oviedo, Spain. A meeting was also held at the IUCr in Hyderabad in 2017. There was overlap with the GA of the IUCR and as there were some matters of importance that were discussed there, the attendance was very low. We discussed mainly the outlook for ECM32 (Vienna) with the local organiser Prof. Kristina Djinovic.

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: Marjolein Thunnissen, Lund, Sweden, Marjolein,Thunnissen@maxiv.lu.se

Vice-Chair: Jan Dohnalek, Prague, Czech Republic, dohnalek@ibt.cas.cz, dohnalek007@gmail.com

Secretary: Ronan Keegan, Oxford, UK, ronan.keegan@stfc.ac.uk