

SIG1: Macromolecular Crystallography

Reported Period: 2018-2019

Report Date: 10 August 2019

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
------	--------------------------------	-----

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

ECA SIG-1 forum: 111.

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 (ECM31)

FOCUS AREA 1 – BIOLOGICAL AND MACROMOLECULAR CRYSTALLOGRAPHY

MS01- Micro & nano crystals in MX

MS02- From data collection to structure finalization: getting the most from your crystal

MS03- Combining methods in macromolecular structure determination, including special conditions MX

MS04- Biophysical characterization and crystallization

MS05- Structural information in drug design

MS06- Molecular machines and big complexes

MS07- Nucleic acids and interactions with proteins

MS08- Membranes and membrane interacting proteins

MS09- Enzymology

MS10- Hydrogen-bonding & weak interactions studied by neutrons and X-rays

MS11- Hot structures in biology

MS12- Structural bioinformatics

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 21st Heart of Europe Bio-Crystallography Meeting at Quedlinburg, Germany, September 20th to 22nd 2018, the 2018 Diamond/CCP4 Data collection and Structure Solution Workshop, 2nd-9th December 2018, Hot topics in contemporary crystallography 2018 (HTCC3), organized by the Croatian Association of Crystallographers, held in Poreč, Croatia, September 22-27 2018, a Magnetic Crystallography course at the International School of Crystallography, Erice, Italy, 31st May to 9th of June, 2018, and the 5th European Crystallographic school held in Stellenbosch, South Africa, 8th to the 14th July 2018.

9. Future/Programmed Activities.

Currently SIG1 is actively involved in the planning of the microsymposia for the forthcoming IUCr Congress in Prague as well as the ECM33 meeting in Versailles, France. Marjolein Thunnissen and Jan Dohnalek are the main contacts from SIG1 for these activities. A list of microsymposia will be 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 ECM32 in Vienna, Austria. A meeting was also held at the ECM in Oviedo in 2018. Much of the discussion at that meeting centred around the increasing inclusion of CryoEM techniques and content in the ECM meeting. It was seen as a good thing given that large overlap with the field of macromolecular crystallography and in the community of users making use of both methods.

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