

SIG1: Macromolecular Crystallography

Reported Period: 2024-2025

Report Date: 19 August 2025

Reported by: Marjolein Thunnissen, Jan Dohnalek and Ronan Keegan

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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: <https://ecanews.org/groups/sig-01/>.

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

SIG1	Macromolecular Crystallography	315 (2021)
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According to ecanews.org

SIG-01	Macromolecular Crystallography	60
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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 : 29

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

SIG1 currently has 315 registered members (from <http://www.xray.cz/eca/eca-sig.asp?id=SIG1>), while meetings are normally attended by ~30-50 individuals. Several dozen 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 (ECM34)

MS1 - Nucleic acids - protein interactions

MS2 - Hot structures

MS3 - Serial crystallography and dynamics/room temperature

MS4 (+SIG-06) - AI, software developments and Machine learning applied to MX and CryoEM

MS5 - Infectious and Neglected diseases

MS6 - Structural studies in Enzymology

MS7 - MX and cryo-EM membrane Protein structures

MS8 - Nucleation and crystal growth/Chaperones and crystallization

MS9 - Large assemblies - using X-rays, cryo-EM and Tomography

MS10 - Structural-based drug discovery

MS11 (+SIG-04) - ED small waves, big ponds – Biomolecules and macromolecules

7. Past Activities other than Microsymposia at ECM

The last ECM meeting took place in Padova in August 2024 and included a range of microsymposia originally proposed by SIG1 (above). Several satellite workshops in biomolecular crystallography also took place at the last meeting. ECA sponsored and supported activities included the Hot topics in contemporary crystallography 2024 (HTCC6), organized by the Croatian Association of Crystallographers held in Dubrovnik, Croatia, from April 7-12, 2024.

8. Future/Programmed Activities.

SIG1 has been actively involved in the planning of the microsymposia for the ECM35 meeting in Poznan, Poland (2025). Ronan Keegan is currently the main contact from SIG1 for this activity. A list of microsymposia were proposed that balance the different interests of SIG1 regarding science as well as methods and instrument development. 2026 is an IUCr International meeting year and no ECM will take place. ECM36 is due to take place in Prague in 2027. Ronan Keegan is the main contact from SIG1 for this meeting and the proposals will be discussed at the ECM35 meeting in Poznan.

A large panel of workshops and courses are foreseen for the coming year. SIG1 has provided letters of support for the 27th Heart of Europe Bio-Crystallography (HEC27) Meeting to take place in Germany in September 2025, the 62nd course of the International School of Crystallography that will take place in Erice in May/June 2026, as well as support for the Central European Course of Computational Structural Biology in Czechia in 2026.

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/>).

9. Other matters. The next annual meeting of SIG1 will take place at the ECM35 meeting in Poznan. It is anticipated that there will be discussion on the microsymposia, chairs and keynote speakers for ECM36 (2027) as well as the election of new SIG officers.

After many years of dedication, both Marjolein Thunnissen (chair) and Jan Dohnalek (vice-chair) have stepped down from their SIG1 roles and replacements should be sought out for them as a matter of urgency.

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

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.

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

Chair (stepped-down): *Marjolein Thunnissen, Lund, Sweden*

Vice-Chair (stepped-down): *Jan Dohnalek, Prague, Czech Republic*

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