

# Minutes for Best Practices 2025 SIG meeting

**Date** Feb 6, 2025 2:00 PM EST

## **Attendees :**

- Johan Hattne
- Dorothee Liebschner
- Nathaniel Michael Barker
- Frances Bernstein
- Herbert Bernstein
- Aaron Brewster
- Lee Daniels
- James C. Fettingner
- Diana Tomchick
- Mitch Miller
- Steven Sheriff
- Allen Oliver
- Danielle Grey
- Kristina Vitale

## **Minutes**

- Review of ACA 2024 sessions, with approximate number of attendees
- Review of ACA 2025 sessions
  - All sessions planned for ACA 2025 have chairs.
- This meeting is held earlier than usual because we need to suggest topics for the upcoming 2026 IUCr meeting. The ACA wants each SIG to propose three sessions by Feb 14; Dorothee Liebschner would like to see at least one session accepted into the program.
- Allen Oliver: List of the IUCr commissions: <https://www.iucr.org/iucr/commissions>.
- Diana Tomchick, attending as a representative of the IUCr's Commission on Biological Macromolecules (CBM): the IUCr is interested in cosponsoring a computational session with the Commission on Crystallography Computing, which may be the commission closest related to this SIG. They are now soliciting suggestions for sessions and speakers, and cosponsoring a session may increase its chance of acceptance.

- The Biological Macromolecules and Synchrotron and XFEL Radiation commissions may also be of interest.
- The IUCr Program Committee requires diversity in session organizers and speakers, in terms of both gender and geographic location [echoed by Allen Oliver].
- Could we merge some small molecule sessions with the Structural Chemistry commission at IUCr?
- Because the IUCr meeting is an international forum, we should reach out to colleagues from Asia and Europe.
- The IUCr is also looking for workshop suggestions, and plenary and keynote speakers.
- Suggested sessions for IUCr 2026:
  - Dorothee Liebschner: one suggestion from the Google form, "Crystallography and structure of graphene", but this may not be sufficiently general for a session at the IUCr 2026.
  - Aaron Brewster: Artificial intelligence in crystallography, or something more focused on structure, as general AI/ML topics may be suggested by many other SIGs as well. In particular: how are AI/ML tools used in current research?
  - Herbert Bernstein: cautions against referring to predicted models as "AlphaFold models" (or even "AI models"), because the field has grown considerably. The important point is that the models are not experimentally determined.
  - Aaron Brewster can provide a summary description and chair suggestions for his proposed sessions.
- Lee Daniels: combining techniques to determine difficult structures, e.g. electron and powder diffraction with AI.
- Aaron Brewster: Serial crystallography.
- Steven Sheriff: Next generation model (and data) validation, and validation metrics, particularly in light of recent predicted models. Validation is an underrepresented topic.
  - Dorothee Liebschner: validation has long been taken for granted, but that does no longer hold with predicted models.
  - Steven Sheriff: the wwPDB may be a good place to start looking for session chairs for a validation session.
- IUCr 2026 sessions, next steps:

- Diana Tomchick: send the session summaries to the chair and the representative of the commission--essentially everybody who may be interested. Dorothee Liebschner will do just that.
- Closing items
  - Dorothee Liebschner: soliciting nominations for chair elect (to become chair) and secretary/treasurer for this SIG. Any plans to try to engage more volunteers for the SIGs?
    - Allen Oliver: there will be more efforts during ACA 2025, such as a booth in the exhibit hall. The ACA council is aware that SIGs would like to reach out, especially to younger attendees.
    - Allen Oliver: in case of concerns, do not hesitate to reach out to the ACA executive committee.
  - Aaron Brewster: would like to run an HDRMX workshop at ACA 2026. Even if it will not become a formal workshop, he would like to secure space for an informal discussion on the topic during the 2026 ACA meeting.