

**Report on the ACA Best Practices for Data Analysis and Archiving SIG meeting,
Jun 11 2024**

The officers of the SIG are:

Chair 2024: Christine Beavers

Chair-elect 2024/Chair 2025: Dorothee Liebschner

Secretary-Treasurer 2024-2025: Jean Jakoncic

During our discussion, a few broad themes developed; they are summarized below and elaborated in the minutes:

1. There is a concern among some members of the BP SIG that open data regulations coming down the pipeline may have repercussions within the ACA community, and we'd best prepare ourselves. A quick search, by the Chair and Co-Chair, of White House communications yielded [this post](#), but it did not give great detail about the implementation or enforcement of any regulations.
2. That AI/ML and Big Data are themes of interest from a number of directions. Dorothee Liebschner proposed a session that explores how predicted models are employed from a programming viewpoint. Our discussion of open data spawned a conversation of how FAIR data is defined and implemented. In light of the 75th anniversary, we discussed a session that focuses on the frontiers of crystallography as they align with AI/ML, but this may become a topic within a transactions session.
3. We did find that there were procedural/organizational questions asked by ACA council members during the meeting that could have been more efficiently handled in an email or after the meeting, if the SIG chairs had been given some advance notice. These questions did not assist the conversation among SIG members and did detract from the meeting flow.
4. The following sessions were proposed for the ACA 2025:
 - a. Predicted Models
 - b. Where is crystallography going: How to take advantage of AI/ML.
 - c. Data Analysis Software
 - d. High Data Rates
 - e. FAIR data in a multi-modal world

Attendance:

- Sara Andres
- Gerald Audette
- Allen Oliver
- Dorothee Liebschner
- Marian Szebenyi
- Aaron Brewster
- Herbert J. Bernstein
- Samantha Powell

- Dorothee Liebschner
- Alexandra Giglia
- Cora Lind-Kovacs
- Jean Jakoncic

This year's attendance (12) was noticeably lower than last year (17)

Minutes:

- Christine Beavers introduced herself and began the slideshow outlining the discussion (appended at the end of the report).
- First order of business, she introduced the other members of the SIG executive,
 - Co- chair Dorothee Liebschner dcliebschner@lbl.gov
 - Secretary/Treasurer Jean Jakoncic, jjakoncic@bnl.gov
- CMB opened the floor to session suggestions:
 - DL suggested a session on new/updated workflows that make use of predicted structures.
 - Gerald Audette came knocking with a mention of the 75th anniversary of the ACA next year, and that a Transactions session on the "Evolving landscape of structural science" would dovetail nicely with Dorothee's suggestion.
 - Allen Oliver asked a question on the number of abstracts in the sessions scheduled for 2024. Since neither the chair or the co-chair had access to the full numbers in Oxford abstracts, this question could only be partially answered (scheduled talks only) by flipping through the session pages in [the schedule](#).
 - Aaron Brewster raised the point that depositing multi-modal data has myriad challenges that are currently unaddressed.
 - Herbert Bernstein apologetically raised the spectre of imminent data sharing regulations coming to force in 2025-2026. His concerns focused on the potential of data loss. CMB agreed to look into the issue further, as her experience at Diamond gave her some insight.
 - AO interjected that this is more of an AIP issue, HB asserts that we need to protect ourselves.
- Second order of business is Chair-Elect nominations.
 - Gerald reminds us that 2026 is a joint ACA-IUCr meeting, and that there may be a lighter burden WRT session organization.
 - AO retorts that there will still be SIG reports required in 2026. Adds that YSSIG and Canadian SIG are happy to co-sponsor sessions and that session proposals are due June 30th.
 - CMB mentions that organization of sessions entirely outside of the ACA is a bit new to her and then returns the discussion to Chair-elect nominations.
 - AB reminds CMB that nomination committees exist. CMB acknowledges this fact.
 - No nominations are tendered; a nomination committee will be needed.
 - AO queried about session sponsorship, which was answered by CMB with what she had seen during their brief foray into Oxford Abstracts- some had sponsors, some did not.

- AB returned the discussion to the ACA's relationship to AIP which evolved into discussing a session on FAIR data. A recent LCLS workshop that AB had organized revolved around Big Data and how to get it into a shareable form. HB adds that AI and Big Data are related. Returning to the FAIR data topic, a session with those well versed in FAIR data (e.g., John Helliwell) would be good for the community.
- Meeting ended

Best Practices SIG

2024 SIG meeting

June 11, 2024

Current SIG officers

CHAIR 2024:
Christine Beavers



CHAIR ELECT 2024/CHAIR 2025:
Dorothee Liebschner



SECRETARY-TREASURER 2024-2025:
Jean Jakoncic



ACA 2024 Sessions

- **Sponsor**

- 1.1.2 Provenance, workflow, and responsibility for X-rays, neutrons, and electrons Pt I
- 1.2.2 Provenance, workflow, and responsibility for X-rays, neutrons, and electrons Pt II
- 3.1.4 Data Analysis Software
- 4.2.4 High Data Rates
- 4.1.1 Structures From Artificial Intelligence

- **Co-sponsor**

- 3.2.2 Serial Crystallography
- 3.1.6 Developments in data collection and automation in MicroED
- 4.1.5 Latest developments, applications and experiences featuring Quantum Crystallography

ACA 2025 Suggestions???

Nominations for Chair elect

As chair-elect (2025), you will:

- Co-organize BP SIG activities for the 2025 meeting with chair
- Stand in for chair if necessary

As chair (2026), you will:

- Attend and advocate for BP SIG sessions at the 2026 ACA planning meeting (held in 2025)
- Facilitate BP SIG activities at the 2026 meeting

Also, together with other members of SIG executive committee:

- Attend ACA planning session (following annual ACA meeting)
- Write annual SIG report for ACA
- Select Etter Student Lecture Award winner

