



# Ronin Institute for Independent Scholarship

Dr. Herbert J. Bernstein, Research Scholar

28 August 2020

## MEMORANDUM

From: Herbert J. Bernstein, Chair-elect Best Practices SIG  
To: ACA Council  
Re: ACA Best Practices SIG Report

This is a report on the ACA “Best Practices for Data Analysis & Archiving SIG” (ACA Best Practices SIG) as of the conclusion of the ACA 2020 virtual meeting. The purpose of the Best Practices SIG is “to further the advancement of all aspects of the application of Best Practices for Data Analysis and Archiving to structural science and to promote communication between persons interested in such techniques and results.”

The officers of the SIG are:

Chair 2020: John Westbrook  
Chair-elect 2020/Chair 2021: Herbert J. Bernstein  
Secretary-Treasurer 2020-2021: Raquel Bromberg

The nominees for Chair-elect 2021/Chair 2022 are Aaron Brewster and Lee Daniels. Both have accepted their nominations with the following statements. We will be asking each of them to send the ACA office a photo and ballot statement for the election.

Aaron Brewster

I'm honored to be nominated as the ACA Best Practices SIG Chair-elect for 2021/Chair 2022. I am a project scientist working for Nicholas Sauter in the Computational Crystallography Initiative at Lawrence Berkeley National Labs, specializing in software development in support of X-ray free-electron laser (XFEL) sources and synchrotron sources. I was first interested in best practices early in the life of XFELs where file formats were not standardized, so I worked with Herbert Bernstein (Dowling College, Oakdale NY, USA), to convert LCLS diffraction data to CBF, using the IUCr ImageCIF standard. Later, as part of the DIALS project (Diffraction Integration for Advanced Light Sources), I worked with Herbert, Graeme Winter (Diamond Light Source, UK), and beamline scientists at SwissFEL and EuXFEL to implement NeXus support for XFEL detectors. The multi-tile detectors at all these facilities have specific geometries that require precise representation by way of extensive metadata, suitable for representation by NeXus. As part of this work, I contributed example XFEL datasets for the NeXus 'Gold Standard' paper in Acta D that will serve as a reference for XFEL and NeXus in the data standards and beamline communities. As Chair-elect, I will bring this

experience to help the ACA continue to enact policies and recommendations for best practices in computational crystallography.

Lee Daniels

My recent move to an organization responsible for crystallographic data archival fits my career-long interest in reliable data access, from historical to those not yet produced. So I was pleased to see the ACA step up to support best practices for data analysis and archiving, and to see the movement among scientists and manufacturers to support FAIR (findable, accessible, interoperable and reusable) data standards. As our probes expand beyond x-rays and neutrons (i.e. microED and cryoEM, for now), we may need to be broad-minded in our ideas about data, encouraging coordination and collaboration, guaranteeing reliable data and archival practices. We need to be open to innovation, as techniques evolve at an ever-increasing rate. Fortunately, our new world of communication has enhanced the adoption of standards (and their improvement). Structural scientists have the advantage of decades of experience in handling "large data", so our contribution to the larger world of data can be significant to science in general. Thus the Best Practices for Data Analysis and Archiving SIG arrived at a most opportune time, and I look forward to a chance to be more directly involved in the process.

The sessions that had been scheduled in 2019 for the 2020 meeting for which the Best Practices SIG would have been responsible were a morning session on Meeting the Challenges of Raw Data Deposition with Wladek Minor as Chair and a satellite workshop for software developers on the new PDB mmCIF-based coordinate deposition requirement and on how software developers could make it easier for depositors to get it ready for deposition with John Westbrook as organizer. Unfortunately due to CoVID-19 and the reduced virtual meeting schedule, the proposed session and workshop were not held. However, I am pleased to report that a successful e-workshop on a subject related to the cancelled session and to an IUCr XXV workshop on "MX raw image data formats, metadata and validation" was held on 22 August 2020. A report is available at

[http://www.medsbio.org/meetings/HDRMX\\_22Aug20.html](http://www.medsbio.org/meetings/HDRMX_22Aug20.html)

We invite the ACA to bring at least some future best practices workshops under ACA auspices. We will be proposing an e-workshop on High Data Rate Macromolecule Crystallography (HDRMX) in Fall 2020 and a hybrid workshop on Raw and Processed Data Formats (WRPD) at ACA 2021 to the education committee before October 2020. We already have a commitment for modest Dectris sponsorship for future High Data Rate Macromolecular Crystallography (HDRMX) meetings and workshops, and we have a good working relationship with the IUCr COMCIFS (Committee on the Maintenance of the CIF Standard) and IUCr COMMDAT (Committee on Data), as well as with the NeXus International Advisory Committee. Formalizing a long-term ACA involvement in these community efforts would seem to be in everybody's interests.

There was a Best Practices SIG virtual meeting during ACA 2020 on 14 August 2020. The Chair, John Westbrook, and the Chair-elect, Herbert J. Bernstein, agreed to have the Chair-elect chair this session. Minutes were taken by the Secretary-Treasurer, Raquel Bromberg, as follows:

## **Minutes – Meeting of the Best Practices SIG – Friday, August 14, 2020**

The meeting of the Best Practices Special Interest Group convened at noon EST Friday, August 14, 2020 during the 70<sup>th</sup> Annual Meeting of the American Crystallographic Association, intended for San Diego, CA but held online due to COVID. The points of agenda included:

- Report from 2019 by John Rose
- discussion of sessions and workshops for the 2021 sessions;
- discussion of the upcoming elections and the selection of candidates for the chair-elect position;
- old business;
- new business

Attendance was not taken, but there were ~20 members participating in the discussion and included among others (in alphabetical order): Herbert Bernstein (chair-elect), Dominika Borek, Raquel Bromberg (secretary), Joe Ferrara, Andy Howard, John Rose, Nicholas Sauter, and Diana Tomchick.

[1] Permission to record was requested

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No one objected. The meeting was recorded.

[2] Possible sessions and workshops for 2021 were discussed

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Being one of the last SIG meetings to take place, several relevant sessions were already proposed by BIOMAC. These included: Computing & Data Management (CDM), Meeting the Challenges of Raw Data Deposition (MCRD), What can and can't we see reliably at resolution X (WCWS), and Improving Existing Structures (IES). Herbert Bernstein is a chair of CDM. Jane Richardson is a chair of WCWS. Andy Howard is a chair of IES.

Two workshops were also already proposed: Workshop on Raw and Processed Data Formats (WRPD) for ACA 2021 and HDRMX online workshop for Nov 2020. Herbert Bernstein is a chair of WRPD. Jean Jakoncic and Dale Kreidler are chairs of the HDRMX workshop.

WRPD will be hybrid (online and in-person). It will broadly cover all relevant data formats, raw and processed.

The HDRMX workshop will also cover electron diffraction. Andy Howard volunteered to recruit a second chair for the electron diffraction component. Target date for the workshop: Nov 2020.

Bernstein noted the need for every session to have at least two chairs in order to have a chance of being approved, even if those chairs might be swapped out for someone else later. Andy Howard recommended Christine Zardecki as the second chair for IES. Howard also recommended that WCWS include cryoEM.

Dominika Borek suggested an additional session for detectors, to be co-sponsored by the BIOMAC, cryoEM, and small molecule SIGs, with the Best Practices SIG as the primary proposing SIG. It would cover how detectors are built, how fast they collect data, what to do when collecting data very fast, how they perform for small/large molecules, etc. Diana Tomchick suggested the name: "Advances in Detector Technology" (ADT). Joe Ferrara volunteered to be a chair. Dominika Borek suggested finding someone from GATAN, FEI, Dectris, etc. to be the second chair and promised to

email Herbert Bernstein suggestions by Sunday, August 16, 2020, 11PM EST. She also volunteered to check with the other SIGs to see who wants to co-sponsor the session.

Nicholas Sauter broached the formal business plan necessary to get a workshop approved. Herbert Bernstein confirmed that October 1 is the deadline for the workshop paperwork and Sauter promised to volunteer someone from his group by Sunday for the workshop planning. [Subsequently, Nicholas Sauter recommended Aaron Brewster as a co-chair of the HDRMX workshop, and Aaron accepted]. The HDRMX workshop will require a smaller budget and be easier to plan due to being entirely online.

Priorities were assigned to the sessions for the planning meeting in the following order, with no objections: CDM (1), MRCD (2), ADT (3), WCWS (4), and IES (5).

[3] The discussion of the upcoming election of the chair elect

Herbert Bernstein, chair-elect for 2020, will be chair in 2021. Aaron Brewster is a nominee for chair-elect 2021. ACA prefers at least two candidates. Joe Ferrara recommended Lee Daniels as second nominee for chair-elect.

[4] Old business

No objections were raised to John Rose's report from 2019.

[5] New business

Nothing was raised.

The results of these discussions were used both to provide the chair-elect 2021 nominations confirmed above and to inform the 2021 Program meeting in which the Chair-elect participated. The two highest priority Best Practices sessions, Computing & Data Management (CDM), Meeting the Challenges of Raw Data Deposition (MCRD), were accepted for the 2021 meeting in the 2021 Program meeting.

Activities between now and the ACA 2021 meeting will be finishing arrangements for the election of a Chair-elect, organizing two workshops, and working with other SIG chairs and ACA headquarters to ensure that arrangements for the sessions in which the Best Practices SIG is either the lead or a co-sponsor are in good shape.

Respectfully Submitted,



Herbert J. Bernstein  
Best Practices SIG Chair-elect