



Ronin Institute for Independent Scholarship

Dr. Herbert J. Bernstein, Research Scholar

17 August 2021

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 2021 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 2021:	Herbert J. Bernstein
Chair-elect 2021/Chair 2022:	Lee Daniels
Secretary-Treasurer 2020-2021:	Raquel Bromberg
Chair 2020:	John Westbrook

The nominee for Chair-elect 2021/Chair 2022 is Aaron Brewster.

The sessions in ACA 2021 in which the Best Practices SIG was involved were:

2.2.2 Computing & Data Management Tuesday, 8/3/2021 @ 12-3 PM EDT Chair(s): Herbert J Bernstein & Dale Kreidler, Sponsoring SIG: Best Practices, Co-Sponsoring SIG: Bio

3.1.1 Advances in Detector Technology Wednesday, 8/4/2021 @ 12-3 PM EDT Chair(s): Joseph Ferrara & Christopher Russo, Sponsoring SIG: Cryo EM Co-Sponsoring SIG: Best Practices

4.2.2 Meeting the Challenges of Raw Data Deposition Wednesday, 8/4/2021 @ 12-3 PM EDT Chair(s): John Rose & Wladek Minor, Sponsoring SIG: Best Practices, Co-Sponsoring SIG: Bio

4.2.3 Sample Prep for Cryo-EM and Crystallography Sunday, 8/1/2021 @ 12-3 PM EDT Chair(s): Edward Pryor, Sponsoring SIG: Cryo EM, Co-Sponsoring SIG: Best Practices

Best Practices had also proposed a Gold Standard Workshop, but that was not included in the final virtual ACA 2021 schedule in view of the continuing pandemic and the need for ACA 2021 to be virtual. However, I am pleased to report that a related HDRMX workshop was

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successfully held as a day-0 virtual workshop at IUCr XXV on 14 August 2021. We once again invite the ACA to become involved in these community efforts. 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 2021 on 28 July. Minutes were taken by the Secretary-Treasurer, Raquel Bromberg, as follows:

Minutes – Meeting of the Best Practices SIG – Wednesday, July 28, 2021

The meeting of the Best Practices Special Interest Group convened at noon EST Wednesday, July 28, 2021 during the 71th Annual Meeting of the American Crystallographic Association, held online due to COVID. The points of agenda included:

- Welcome
- Nominations for 2022
- Proposed Sessions for ACA 2022 in Portland
- Old Business
- New Business

Attendance was not taken, but there were ~20 members participating in the discussion and included among others (in alphabetical order): Oskar Aurelius, Herbert Bernstein (chair), Dominika Borek, Derek Bratcher, Aaron Brewster, Raquel Bromberg (secretary), Lee Daniels (chair-elect), Ana Gonzalez, Thomas Grant, John Helliwell, Wlodek Minor, David Rose, John Rose (ACA President), Peter Stephens, Diana Tomchick (ACA Vice President), and Mary Ann Wu.

[1] Permission to record was requested

No one objected. The meeting was recorded.

[2] Each attendee briefly introduced himself/herself

[3] Nominations for 2022

Herbert Bernstein (chair) requested nominations for the 2022 chair-elect. This individual would be chair in 2023. There were no nominations or volunteers. Bernstein nominated Aaron Brewster. Lee Daniels seconded the nomination and Brewster accepted. Bernstein requested that any additional nominations be sent to his email.

Bernstein requested nominations for the 2022/2023 secretary treasurer. There were no nominations or volunteers.

[4] Proposed Sessions for ACA 2022 in Portland

Bernstein proposed two sessions:

- Crystallography in the era of highly accurate models from sequences
- Advances in XFEL and synchrotron serial crystallography

Brewster asked about the parameters or subtopics of the sessions in terms of standards. Bernstein stressed the importance of knowing what we mean by a “highly accurate” model; what is the validation level and quality standard that a model should be taken to before it is used in molecular replacement for solving a structure. A lot of people are currently moving toward this; collect data and immediately get the sequence space model and try to do molecular replacement.

John Helliwell questioned the wording “highly accurate.”

Wladek Minor indicated that the session would be interesting but that its quality and value would depend on who was chosen to speak. He added that there is a fair amount of misinformation regarding these methods and also that it is very difficult to convince people to be speakers.

Diana Tomchick shared that many other SIGs are also interested in sessions related to AI, machine learning, AlphaFold2, and so if anyone is worried about not getting enough speakers, they could consider contacting the other SIGs to co-sponsor a session. Bernstein said they should definitely consider co-sponsoring with BIOMAC SIG.

Minor asked Tomchick how many people are attending the ACA and she answered ~600 registered and over 300 abstracts submitted.

Bernstein asked for one or two nominations for chairs for the proposed sessions. For Crystallography in the era of highly accurate models from sequences, there were no volunteers and Bernstein nominated Brewster as the chair. Minor volunteered to be the co-chair. Bernstein asked that the chairs come up with a proper title, write a descriptive paragraph, etc.

Bernstein remarked that because a lot of exciting things are happening in serial crystallography both in XFELs and synchrotrons, it would be wise to have a session about it. There was limited enthusiasm regarding this session.

Lee Daniels suggested a third session: We need to have archival ability to store data far into the future. So the session would be on data archival strategies for the future. Daniels would be willing to co-chair the session. John Rose volunteered to co-chair the third session with Daniels.

Bernstein asked for one more session. John Helliwell suggested another data archiving session that would be a follow-up session of the chemical crystallography session that will be happening at the IUCr conference. It was ultimately decided to merge the suggestion into the data archiving session already proposed, but to make it a full-day session with the following tentative title: Data archiving strategies for MX, Chem. Cryst., Cryo-EM, Powder, MicroED. Brewster suggested that a worthwhile goal of the session would be producing actionable recommendations to funding bodies, and having a panel for the session. Minor suggested inviting people from NIH in that case.

In terms of popularity, Bernstein ranked the XFEL/synchrotron session as third priority and asked for a chair. There were no nominations or volunteers and Bernstein nominated himself as a chair. The Crystallography in the era of highly accurate models from sequences session was put in first place for session rankings, and the data archiving session was ranked as second.

Bernstein again asked for a recommendation for a fourth session. Mary Ann Wu suggested a session on Hardware standardization in structural biology. Bernstein asked for a chair. There were no nominations or volunteers. Minor suggested it be changed to Hardware and Software Standardization in Structural Biology. Tomchick suggested that the chair be selected from someone who did not attend the SIG and Bernstein chose Andreas Förster [unfortunately, as we later learned, recently deceased].

[5] Discussion of Secretary/Treasurer

Daniels suggested nominating someone to be the nominating committee. Bernstein nominated Raquel Bromberg (the current secretary/treasurer) to be the nominating committee of the secretary/treasurer and she accepted.

[6] Old business

None

[7] New business

Tomchick (ACA Vice President) announced she is in charge of next year's Transactions Symposium. The current title is: The Contributions of Structural Science to Tackling a Pandemic: COVID-19 as a Paradigm. She is asking the various SIG if they would like to co-sponsor the symposium and if they wish to nominate a speaker or multiple speakers for consideration to speak. She asked that suggestions be sent to her email address or through the SIG chairs, and also said that the Best Practices SIG could contribute because of the amount of data that has been generated, both sequence data and diffraction data that have been made available for people for all kinds of research, and so it would be great to have the SIG's co-sponsorship. It wouldn't take away any of the co-sponsorship or sessions that the SIG already proposed because the symposium will happen regardless. Bernstein strongly recommended co-sponsorship and there were no objections. Tomchick requested speaker suggestions and volunteers to assist with organizing the symposium.

We are pleased to report that all of the proposed sessions made it through the planning session, with Crystallography in the era of highly accurate models from sequences co-sponsored with Bio, and Hardware and Software Standardization in Structural Biology co-sponsored with Light Sources. Aaron Brewster remains chair of the former, co-chair to be selected by BIO. Martin Fuchs and Raquel Bromberg to be chairs of the latter.

Activities between now and the ACA 2022 meeting will be finishing arrangements for the elections, organizing more 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. The current chair will be handing off responsibility for those activities to the chair-elect, Lee Daniels, as of 2022, but hopes to remain involved in the activities of the Best Practices SIG well into the future.

Respectfully Submitted,



Herbert J. Bernstein
Best Practices SIG Chair