SIG Report
Best Practices for Data Analysis and Archiving
30 August 2022

From: Lee Daniels, Best Practices SIG Chair
To: ACA Council
Re: ACA Best Practices SIG Report

We here report the activities of the ACA "Best Practices for Data Analysis & Archiving SIG" (Best Practices SIG) following the SIG online meeting held 20 July 2022 .

The officers of the SIG are:
Chair 2022: Lee Daniels
Chair-elect 2022/Chair 2023: Aaron Brewster
Secretary-Treasurer 2022-2023: Charles Hespen
Chair 2021: Herb Bernstein

The purpose of this 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." As structural science expands and modern techniques bloom, the SIG provides a common area for diverse ideas among all these technologies. We aspire to consider both the past and the future of structural sciences and the data available to the community, and to encourage the open discussion and action on keeping these techniques and data viable in the future.

For the 2022 ACA Meeting in Portland, OR, the Best Practices SIG sponsored/co-sponsored the following sessions:
- 1.1.2 Use of AI predicted Models in Structural Biology/Crystallography (Saturday 30 July, 08:30 - 11:30 Salon F) – co-chairs Aaron Brewster & John Moult
- 2.2.4 The Future Of Past Data For Single Xtal , Cryo EM, Powder & Micro ED (Sunday 31 July, 14:00 - 17:00 Salons C D) – co-chairs Lee Daniels & John Rose
- 4.1.2 Hardware and Software Standardization In Structural Biology (Tuesday 2 August, 08:30 - 11:30 Salons A B) – co-chairs Martin Fuchs & Raquel Bromberg
- 4.2.1 Advances in XFEL and Synchrotron Serial Crystallography (Tuesday 2 August, 14:00 - 17:00 Salon E) – co-chairs Herb Bernstein & Aaron Brewster

The Best Practices SIG met online on July 20, 2022, prior to the Portland ACA meeting.

Upon approval of the 2021 minutes, the SIG moved to nominations for the 2023 chair elect (2024 chair). A call for volunteers did not produce any nominees, so a nominating committee was formed, including the current chair (Lee Daniels), chair-elect (Aaron Brewster), secretary-treasurer (Charles Hespen) and a volunteer member John Rose. As of this writing one member, Christine Beavers, has agreed to stand for the position. The nominating committee expects to determine whether other nominees are willing to stand by 31 August. The Secretary/Treasurer position is a two-year term; our current office holder, Charles Hespen, will serve in both 2022 and 2023 in this position so no nominations are required this year

The chair then opened the floor to proposals for sessions for the 2023 ACA meeting in Baltimore.

- Krzysztof Wozniak (Univ. of Warsaw) had submitted a proposal in advance for a session on Quantum Crystallography – Wozniak volunteered to chair, and has confirmed his co-chair as Yu-Sheng Chen (APS, Chicago)
- John Rose proposed a session on "Validating models from the data, other data, and theory" and volunteered to chair the session. Joseph Ferrara has agreed to co-chair the session. Rose proposed this as a possible full day session, split among various techniques
- Aaron Brewster proposed an AI Structure session, possibly co-sponsored by the BioMAC SIG. Two possible sessions based on results vs application
- Herbert Bernstein suggested a session covering current data analysis software – are we properly archiving these results? Also access to raw data? Also consider unmerged data. This could be a workshop if software authors/vendors are willing to participate. Marian Szebenyi volunteered to co-chair this session
- Aaron Brewster also proposed a session on serial crystallography, especially due to the recent emergence of the use of this technique among the small-molecule community. Possible co-sponsorship by the Light source SIG, BioMAC SIG, also Small Molecule. Brewster offered to co-chair this session, and Jennifer Wierman agreed to co-chair.

The floor was opened for discussion of new business.

John Helliwell and David Rose suggested that future discussion be given to a current UNESCO proposal concerning the availability of raw data, the question of data ownership, and the status of "open science."

Aaron Brewster and Herbert Bernstein raised a question about data formats, especially the NeXus standard. Suggested a review of what should be considered mandatory data items, etc.

The meeting was closed on time, within the one-hour time scheduled.