To: ACA Council c/o Kristin Stevens (kstevens@hwi.buffalo.edu)
From: Executive Committee, Scientific Interest Group on Best Practices for Data Analysis and Archiving
Re: Annual Report
Date: 8 August 2018

Our newly-formed SIG conducted its first business meeting on July 21, 2018 at the Toronto ACA meeting.

- Executive committee: Nicholas Sauter (Chair, nksauter@lbl.gov), John Rose (Chair-Elect, jprose@uga.edu), and Suzanna Ward (Secretary-Treasurer, ward@ccdc.cam.ac.uk).

- Poster 168 was presented by John Rose to introduce the SIG, amplifying the founding mission statement published in the Winter 2018 Reflexions newsletter.

- Elections: A new Chair will be elected in Fall 2018 to replace Dr. Sauter who will term out. We thank our nominating committee (Johan Hattne, hattne@ucla.edu and Ana Gonzalez, ana.gonzalez@maxiv.lu.se) for identifying two excellent candidates who have agreed to stand for election:

  - **Dr. John Westbrook** (Data & Software Architect Lead, RCSB, Rutgers University, john.westbrook@rcsb.org). Field of interest: Archive management and access.
  - **Dr. Brent Nannenga** (Assistant Professor of Chemical Engineering, Arizona State University Brent.Nannenga@asu.edu). Field of interest: Protein engineering and methods development using crystallography and cryo-electron microscopy.

- 2019 Session at ACA meeting, Covington KY. The Council approved, and the 2019 planning meeting accepted, our proposal to organize a Transactions symposium, with peer-reviewed proceedings to be published as open-access articles in a special issue of *Structural Dynamics.*

  - Title: **Data Best Practices: Current State and Future Needs** (revised from earlier draft)

  - Session chairs: Nicholas Sauter, John Rose, and Talpady Bhat

  - Co-sponsoring SIGs: Industrial, CryoEM, BioMac, Lightsource, SAS, and General Interest

Topics and speakers

Clemens Schulze-Briese	Dectris	Detectors/image formats
Michael Wall	LANL	Analysis and Modeling of Diffuse X-ray Scattering Data
Stephen Burley	Rutgers	The Living PDB
Nadia Zatsepin	ASU	Optimizing Data Quality in Injector-Based Serial Millisecond Crystallography
Wladek Minor	U Va Medical School	Image Archival
John Helliwell	University of Manchester	Developing IUCr standards
Meitian Wang	SLS	SLS data storage/archival
Thomas Proffen	ORNL	Neutron Diffraction
Rama Ranganathan	U Chicago / BioCARS	Electric-field stimulated protein dynamics
Amy Sargeant	CCDC	Challenges and Opportunities Surrounding the curation of small molecule data
Herbert Bernstein	RIT / BNL	Best Practices in Image Clustering for Polymorphs and Dynamics
Brent Nannenga	ASU	Method developments in MicroED

CryoEM (TBA)	TBA	

- o Unresolved issues: we have yet to identify a speaker to represent the CryoEM field.

- o Announced date: This will be an all-day session on Sunday, July 21, 2019.

- o Fundraising. Anticipating that publication charges alone will be $14,000, we would like to work closely with the ACA Council in the coming year to identify funding sources.

- Co-sponsored sessions. The Data SIG has offered to co-sponsor the following:

  - o CryoEM: micro-Electron Diffraction (Brent Nanennga)

  - o BioMac: The Meaning of Resolution (Zbyszek Otwinowski)

  - o BioMac: Radiation Damage in X-ray and EM (Dominika Borek & Gerd Rosenbaum)

  - o SAS: Biomolecular SAS Data and Model Validation and Integrative Biology. Greg Hura, Jill Trewhella.