

Activities of the Biological Macromolecules Scientific Interest Group of the American Crystallographic Association, 2010

Planning for the BioMac contribution to the Chicago meeting began in earnest at the 2009 Toronto meeting. Prior to that meeting, email solicitation of ideas for topics, in addition to proposals by the 2010 SIG chair, led to ideas that were fleshed out at our annual BioMAC SIG organizational meeting. Resulting from these discussions, our SIG decided to individually sponsor ten sessions and co-sponsor with the synchrotron, young scientist, and small angle scattering SIGs, five additional sessions for the 2010 Chicago meeting. The sessions for this meeting planned were: Exciting Structures, Computational: Software Integration and Databases (co-sponsored with Young Scientists SIG) Protein Expression, Purification, Crystallization (How did get a good diffracting xtal?, Long Wavelength Phasing, Radiation Damage (Limit, misinterpretation)(w/Synchrotron SIG), Macromolecular Complexes and Assemblies, Cardiovascular Disease Session (w/Industrial SIG), Molecular Motors and Transactions: In Memory of Bob Bau (In particular, our members are interested in determination/visualization of hydrogen atoms in crystallography and two sessions on Structural Enzymology dealing with biophysics and biology respectively. All of these were accepted for the program in Chicago. However, as consequence of a desire to have a memorial session for Louis Delbaere, the crystallization session was dropped and J Allingham volunteered to chair the memorial session.

There were three workshops organized and presented in Chicago focusing on topics of interest to BioMac SIG members. Gerard Bricogne and colleagues from Global Phasing presented a structural solution and refinement workshop focusing on Buster etc. John Rose and BC Wang presented a workshop on Sulfer-SAD phasing and the CCP4 crew headed by Charles Ballard presented a refinement and graphic session centered on CCP4 tools. Each workshop was highly subscribed with over 30 participants involved in each even through the typhoon-like weather and transportation to the off-site location. Considering that each of these three workshops were in virtually direct competition based on the BioMac demographic, we consider that turnout to be exceptional.

Ed Collins, Mark Wilson, and John Rose chose Kyrstal McLaughlin (University of Rochester School of Medicine and Dentistry) as the BioMac SIG Etter Student speaker for her work on the mechanism by which REX senses the redox environment and presented her talk in the Exciting Structures session. The Structural Enzymology session was very successful this year with many, many abstracts and as a result, we decided to expand these two session to a third session next year. All Biomes-related session chairs have all done a superb job organizing this year's sessions, identifying excellent speakers. Thus far, all of our SIG's sessions have been very well attended.

The SIG leaders continue to have a concern that the large size of the BioMAC SIG group makes it difficult to reach a consensus that accurately reflects the desires and needs of the whole community. Perhaps as a result of this size, a certain level of apathy appears to exist. As in the past two years, the SIG officers began to raise money for refreshments at the BioMac planning meeting. However, because of refreshments to be offered at the poster session, we decided to eliminate food and finish the meeting quickly to attend the poster session.

The present BioMac SIG chair (Ed Collins) would like to thank all the session chairs that contributed so much to the success of the 2010 Chicago meeting. We will be looking for nominations for the 2011 chair-elect from SIG members during the coming months.

Planning for the 2011 ACA meeting. Planning for the 2011 ACA meeting is well underway and being ably led by John Rose and Mark Wilson. Even though we had a small group at our BioMac SIG planning meeting, they were vocal in their wants and concerns; we were still able to have a very productive SIG planning meeting to develop various possibilities for sessions that we would like to sponsor for the New Orleans meeting. The outcome of this meeting was a list of 10 session topics that we would like to sponsor: 1) The use of databases in structural biology (Wladek Minor chair), 2) Collecting good data with microcrystals (asking Alex Soares and Dominca Borek), 3) PSI contributions to the home lab (Steven Sheriff chair?), 4) Structural enzymology I, spectroscopic and other complementary methods (Allen Orville chair), 5) Structural enzymology II, mechanistic (chair TBD), 6) Structural Enzymology III, biological implications (Chair TBD), 7) Crystallization (asking Alex McPherson), 8) Macromolecular Assemblies (tbd) and membrane proteins (Peter Horanyi and asking Michael Weiner). We have a new idea to present for sessions 9 and 10. We would like them to be a morning and afternoon session on 9) data processing and 10) structural solution in a mixed presentation/workshop style. The idea is that we will provide images for processing prior to the meeting with instructions to process the data and determine structures as well as they can at home. At the meeting, the solutions will be done for them by the

program's developers. At this point, we have a plan to ask Jim Pflugrath (d*trek), Wladek Minor (HKL3000) and Wolfgang Kabsch (XDS) for the morning and representative from CCP4 (refmac5), Gerard Bricogne (buster) and Alex Brunger (cns) and Paul Emsley for Coot to finish in the afternoon. It would be a way for people to try to perform the tasks with real data and a chance to get a fast presentation of how the experts would do it. The chairs for the sessions would be Ed Collins and Andy Torelli (Young scientist). My goal is to ask each of these presenters to have themselves or someone who works for them available after the sessions to "tutor" students who have quick questions. There are a number of different outcomes possible from such an exercise. One of our goals is to write a manuscript describing the results obtained by the participants before attending the session and as given by the authors of the scripts themselves to allow us to compare results obtained that are a result of user intervention.

We believe this number of sessions will increase in our further discussions with other SIGs. There was a great deal of concern discussed by the Biomac attendees that the average age of the meeting participants seems to be trending higher. This is one of the reasons for making two of our sessions be more "hands on" and teaching than are presently done. There was a suggestion to increase the number of students and postdocs presenting during the sessions. There was also a suggestion to just not have a meeting during the years that the IUCr meet to avoid conflict and the expense of going to two large meetings in a year. The council president asked for us to discuss specific areas in which the ACA is not addressing, but nothing was offered. The SIG chair asked for participants to think about it and if they come up with something to share during the meeting.