

Small Molecule SIG Annual Report 2011

2010 Chicago meeting sessions sponsored/co-sponsored by the Small Molecule SIG

07.02 Non-ambient Environments for Specialized Experiments

07.06 Absolute Structure Determination; where are we now?

07.10 Data Collection Strategies (Service, Small Mol)

02.03 Blast from the Past: What was Old is New Again

05.01 Cool Structures

07.26 Handling Disorder in Crystal Structures

Sessions were well attended with the possible exception of 07.26, which suffered the usual decline in attendance as a result of being the last session of the meeting. Cool Structures continues to be a popular session in terms of both attendance and submitted abstracts and in particular has a long history of supporting students and allowing them to present their work.

2011 Etter Student Award

The Small Molecule SIG selected John Sander, University of Iowa, as the recipient of the 2011 Etter Student Lecturer Award.

Combined annual meeting with the Service Crystallography SIG

At the 2009 Toronto meeting it was proposed that both the Small Molecule and Service Crystallography SIGs hold 'joint' meetings, given that there is a very large overlap between the membership of both SIGs. This was approved by both SIGs, and tested in 2010. There is some apparent confusion over what exactly is meant by a "joint meeting" of both SIGs. We wish to make clear to Council that it is *not* intended to be a combination of both SIGs, holding one meeting with one chair. Rather, it is an hour of "back-to-back" SIG meetings, starting with the Service Crystallography SIG meeting and, when that closes 30 minutes later, the chair of the Small Molecule SIG then opens the meeting for the next half hour. Thus: one hour, two meetings. We make this distinction since although the membership is broadly the same, the scientific and practical aims and interests of the SIGs are quite different. The idea of combining them to be held consecutively was born largely of convenience to the membership, so that we only took up one lunchtime of the meeting, and that this would follow a suitable session e.g. Cool Structures, which will be attended by most of the membership anyway.

At future ACA meetings, the Service Crystallography and Small Molecule SIG meetings should be held back to back, starting with the Service meeting, and listed as such in the conference program.

Issues from 2011 Meeting

1. The SIG is sponsoring several sessions this year, *viz*:
 - a. 08.01: *In situ* Diffraction Studies.
 - b. TR.01: Transactions - Time-resolved and Charge Density in Honor of Philip Coppens.
 - c. 05.01: Cool Structures.
 - d. 05.02: Modern Aspects of Crystal Engineering.
 - e. 08.01: Small Molecule Molecular Machines.

As of the time of writing (June 1 2011) all sessions have been very well attended and in some cases the room allocated was too small for the audience. This is noted below. Cool Structures, in particular, attracted so much interest that an extra half day session was added to the program.

2. The SIG noted that hotel rooms are now provided with wireless internet as part of the room charge, a welcome development on previous years.
3. The SIG again requests that a complete, searchable PDF of abstracts be made available on the ACA website in advance of the meeting. Currently each abstract is only downloadable individually as a PDF file.
4. Allen Oliver, Amy Sarjeant and Charlotte Stern were successful in a bid to organize summer schools in crystallography in 2012—2015. The SIG asks if an ACA fund may be set up in order to offer bursaries or some other form of financial support for teaching schools. It was proposed that the ACA membership application or renewal form include an option for members to donate to this fund, in the same way as we now can donate to the various award funds.
5. The issue of the cost of attending the ACA was again raised, especially in the context of the rather small number of Small Molecule students attending the meeting. It was noted that American Chemical Society meetings cost considerably less for student attendance. It was also noted that several poster boards, in all sessions, were empty, and the question was asked if this was a result of students unable to pay to come to the meeting. The 2012 meeting is one day shorter, ostensibly to save money on hotel bills. However the SIG felt more strongly that the question of the meeting location itself - i.e. expensive corporate hotels - may need to be revisited. This is of particular note given that the 2014 IUCr meeting will be held in Montréal; many members of the SIG have very limited, fixed travel budgets and are more likely to attend the IUCr meeting than an ACA meeting, if forced to make a choice.

The Small Molecule SIG requests that Council give serious consideration to hosting future ACA meetings at less expensive venues such as a university campus. Many large universities now have excellent conference facilities and very large exhibition facilities, as do many smaller towns; Council should not dismiss them out of hand.

6. During the course of the meeting members of the SIG raised complaints about the size and layout of several of the rooms used for symposia. Some were much too small, with attendees unable to get in. The layout of another - a long hallway type room with a large pillar effectively blocking a quarter of the space - was entirely unsuitable. We note, however, that most of the plenary lectures were moved to a larger, more suitable room.
7. The poor layout of the poster boards is also a concern. One member commented that the impression one got was that the scientific discussion was almost a sideshow to the commercial exhibit. The poster board area was much too small and congested, and loud, for proper discussion to take place. It did not help that some of the empty space was taken up with a food table and drinks bar, nor that there was a physical barrier (a curtain) erected between the poster area and the exhibit area.

Proposed topics for 2012 meeting

Transactions Symposium: Transformations and Structural Oddities in Molecular Crystals - Honor of Bruce M. Foxman. Co-organizers: Graciela Diaz de Delgado, Magali Hickey, and Kraig Wheeler. The Service Crystallography, M/N/P and General Interest SIGS strongly support this. The themes of the Symposium have already been identified, has have potential speakers.

Crystallographic Information in Pharmaceutical Research and Development. Co-chairs: Magali Hickey and Matt Peterson. This will be co-sponsored by the Industrial SIG. Full day requested. Topics and speakers for this session have already been identified, and it is hoped that it will attract much interest from industrial crystallographers and scientists.

Cool Structures. Co-chairs: Xiaoping Wang and Jeanette Krause. Full day requested, given the popularity of the session this year.

Important Science from Small Molecule Structures. Co-chairs: Larry Falvello and Alberto Albinati. Full day requested.