

Industrial SIG Activity Report: 2011

Chair: Paul Swepton



The ISIG meeting was held Thursday June 1 at noon at the Sheraton Hotel in New Orleans. It was supposed to be held at noon but since the meeting that was using the room prior to the ISIG meeting ran over by 30 minutes, the meeting actually started in the hallway. Note to ACA organizers: please tell session chairmen to keep on schedule. In this case there had supposedly been an equipment failure but the speakers were still being allowed to take questions in spite of the session running over.



Once inside the room we gathered a few more members who had been attending the previous meeting. We had 13 attendees (including the photographer/chair) that

was a bit of an increase over the previous year. There was a good mix of interest between small molecule and macro people that was different from 2010.

ACA 2011

Industrial SIG Meeting Minutes

6/1/2011 at 12:00 pm in room D2-D3

Prepared by Herb Klei

Adhoc secretary

Paul Swepston, the current Industrial SIG chair, called the meeting to order at 12:30 pm (the previous session ran well over their time slot). No formal minutes were available from the 2010 Industrial SIG meeting from the Chicago, IL ACA because the secretary was unable to attend this meeting. The gist of the discussion at the Chicago Industrial SIG meeting was on what type of session would generate the most interest in terms of both attendance and willingness to organize. The consensus was to hold something along the lines of the annual Protein Structure Determination in Industry (PSDI; <http://www.psdi2010.org/psdi2010/programme/proteinproduction.html>) meeting held in Europe. To this end, the afternoon session 03.01, Challenges and Opportunities in Structure Based Drug Discovery, chaired by Nikolay Chirgadze was hosted by this SIG. It was well attended.

Thirteen members attended the Industrial SIG meeting. Attendee affiliation included Cambridge Structural Database, small business owners – some with an academic affiliation, small pharma (Alkermes), and large pharma (Bristol-Myers Squibb, Merck). One of the local program chairs for the Boston ACA, Bruce Foxman from Brandeis University (foxman1@brandeis.edu), also attended. A list was passed around for attendees to enter their name and email.

Sessions for 2012 ACA in Boston, MA

Two sessions sponsored by the Industrial SIG were proposed. Paul Swepston will update the attendees and members on the master Industrial SIG distribution list on the outcome of the Friday planning session.

1) Use of Crystallographic information and structure analysis in Pharmaceutical Development (full day)

Co-chairs – Magali Hickey (magali.hickey@alkermes.com) and Matthew Peterson (petersom@amgen.com). Part or all of this session may be co-sponsored by the Small Molecule SIG. Much interest was already expressed in this session from New Orleans attendees. (Appendix 1)

2) Protein Structure Determination in Industry (1/2 day)

Co-chair – Stephen Burley (stephen.burley@xxx.com) and T BD. Via an email to Bruce Foxman, Stephen Burley proposed to focus this session on fragment-based screening. However, the general consensus at the meeting was to leave the topic more open ended. The primary rationale was recent session held by the Industrial SIG and other devoted to fragment-based screening. Other reasons for generality were to appeal to a wider audience within the macromolecular community and to give the co-chairs the freedom to take the session in the best direction based on interest.

Nomination of 2012 officers

Magali Hickey (magali.hickey@alkermes.com) was nominated for, and unanimously approved as, chair elect.

Mark Oliveira (mark.oliveira@alkermes.com) was nominated for, and unanimously approved as, secretary elect.

Conclusion

The meeting was adjourned at 1:15 pm with a sense of relief and cautious optimism. The level of attendance represents an improvement over recent years. Boston is a biotech / pharma / scientific hub and it should be possible to generate interest in terms of organization and attendance. A good showing in Boston should bring increased visibility to, and participation in, the Industrial SIG.

ISIG Sponsored Session New Orleans 2011

Challenges and Opportunities in Structure Based Drug Discovery

Speakers drawn from the pharmaceutical and biotechnology industry and academe will present case studies of the impact of X-ray crystallography on small molecule drug discovery, with particular emphasis on fragment based approaches.

Chair: Nickolay Chirgadze (nchirgad@uhnresearch.ca)



Appendix 1.

Session proposal for the 2012 ACA national meeting to be held in Boston, Massachusetts

Session title: Crystallographic Information in Pharmaceutical Research and Development

Session organizers and chairs: Magali Hickey (Alkermes, Inc.) and Matt Peterson (Amgen, Inc.)

Vision for a full day session:

Crystallography and crystal structure mining have become recognized as powerful tools in pharmaceutical R&D. Progress in the past decade or two is evident in drug discovery as well as in Active Pharmaceutical Ingredient (API) and drug product development. Structural analysis of small molecules (<1000 Da) and large molecules such as therapeutic proteins forms a pillar in advancement of compounds under investigation as therapeutics. Crystal structure determination of large molecules and their complexes with ligands and targets has provided significant advances in drug design and discovery efforts. In the case of small molecule drug candidates, crystal structure determination and analysis spans routine identification of chemical structures, assignment of absolute stereochemistry, guidance in form selection for development, rationalization of kinetic and thermodynamic solubility trends, and understanding molecular interactions of drugs with formulation components.

We invite experts from academia and industry alike to join the discussion on the use of crystallographic data and analysis for molecules in drug development – reflecting on past achievements and future directions. In particular, we are seeking perspectives on how molecular design and materials characterization using crystal structure analysis techniques can yield insights that facilitate understanding of the structure and function of medicines.

Session 1: Design and characterization of molecules in drug development

Chair: Magali Hickey

Proposed topics: Perspective on crystallography and structural information in pharmaceutical development; structure based drug design; crystal engineering and data mining.

Proposed Speakers: Örn Almarsson (Alkermes, Inc.); Dimitri Moustakas (Astra Zeneca); Mike Zaworotko (USF) + 2 open for general abstracts

Session 2: From pharmaceutical form selection to process development

Proposed topics: Structure/property relationships; polymorphism; understanding dissolution behavior; development and scale-up of drug substance; understanding mechanism for hydration/dehydration dynamics

Chair: Matthew Peterson

Speakers: Mark Tawa (Alkermes, Inc); Eugene Cheung (Amgen, Inc.); Peter Wood (CCDC) + 2 open for general abstracts

Appendix 2. ISIG meeting attendees

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