## MS46-T01

#### **Crystallography Hic et Nunc (Quo Vadis revisited).** Katherine A. Kantardjieff. *Department of Chemistry and Center for Molecular Structure, California State Polytechnic University Pomona, California 91768 USA.* E-mail: kantardjieff@csupomona.edu

There is growing concern, particularly in the United States, that education in general is neither training adequate numbers of students for careers in science and technology, nor developing broad scientific and technological literacy that is necessary for full participation in society. In our own field of crystallographic science, recently we have seen high profile and embarrassing retractions in the peer reviewed literature, often the result of pathological science or inadequate review. Academic crystallography has largely migrated from a research specialty to a technique employed by a wide community of users. Few university departments hire faculty capable of teaching crystallography, and formal courses have all but disappeared from course catalogs. Yet, increasingly large numbers of "naïve" users, who require more assistance than the experienced user, work in academia and industry. This has led to the growth of and dependence on independently funded workshops and summer schools in crystallography, aimed at different audiences, as well as an increasing dependence on other, non-traditional curricular resources for instruction that allow crystallography to be selftaught. If crystallographic science is to remain vibrant, and the results of its analyses reliable, how will we instruct and train in ways that attract and retain a broad pool of talented people in the next decade? This talk will explore the current state of affairs in crystallographic science. particularly macromolecular crystallography, and survey the ways that crystallographers are pushing the boundaries of technology to educate and train the next generation of scientists.

Keywords: crystallographic education, macromolecular crystallography, World Wide Web

#### MS46-T02

*RapiData*: A practical course in macromolecular xray diffraction data measurement and structure solving at the NSLS. <u>R.M. Sweet</u>, A. Soares, *Biology Department*, *Brookhaven National Laboratory*, *Upton*, *NY*, USA.

Synchrotron radiation is an indispensable tool for many macromolecular crystallography groups. Some synchrotronspecific skills are learn best in an intensive hands-on training program. To provide such an educational experience, we have designed a course in Rapid Data Collection and Structure Solving, which we have presented twelve times.

The course accommodates nearly 50 students. All students are encouraged to **bring their own specimens** for data collection, and to bring old data for the data-reduction and structuresolving tutorials. The course includes an optional five-hour lecture course on the fundamentals of crystallography, then two days of lectures on detailed aspects of data collection and structure solving. Then for two more days we move to the NSLS for data collection, and concurrent tutorials on the contents of the lectures.

Students are divided into 10 sections. Each section gets a total of about 20 hours on a beamline, including undulator

beamlines if appropriate. A crystal-preparation lab is available for all students, with crystals supplied for those without crystals, and a beamline is available for these students to try their hand at diffraction measurements on sample specimens they will have mounted themselves. The course is sponsored by grants from the US National Institutes of Health, and Department of Energy, and by donations and in-kind assistance from pharmaceutical and equipment companies.

### MS46-T03

Update on the Tutorial for Learning and Teaching Macromolecular Crystallography. <u>Annette Faust</u><sup>a</sup>, Sandra Pühringer<sup>b</sup>, Nora Darowski<sup>b</sup>, Santosh Panjikar<sup>c</sup>, Kay Diederichs<sup>d</sup>, Uwe Mueller<sup>b</sup>, Manfred S. Weiss<sup>b</sup>. <sup>a</sup>Centre for Biochemistry and Molecular Biology (ZBM), Christian-Albrechts-University of Kiel, Am Botanischen Garten 1-9, D-24118 Kiel, Germany. <sup>b</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Macromolecular Crystallography (BESSY-MX), Albert-Einstein-Str. 15, D-12489 Berlin, Germany. <sup>c</sup>EMBL Hamburg Outstation, c/o DESY, Notkestr. 85, D-22603 Hamburg, Germany. <sup>d</sup>Department of Biology, University of Konstanz, Box M647, D-78457 Konstanz, Germany.

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The previously described macromolecular crystallography tutorial [1] has been significantly revised and expanded. Two new experiments (SIRAS and RIP) have been designed to complement the five experiments (S-SAD, MAD, MR, ion binding and ligand binding) of the first edition of the tutorial for learning and teaching macromolecular crystallography. Furthermore, the tutorial has been re-organized and in part rewritten to reflect the comments and suggestions of the users. The most significant overhaul was applied to the data processing part of the tutorial. A major design feature of the tutorial is that all of the utilized proteins used are commercially available; they can be easily and reproducibly crystallized and mounted for diffraction data collection. For each of the seven experiments the raw images and the processed data are provided for learning or teaching the steps of data processing and structure determination.

[1] Faust et al. (2008). J. Appl. Cryst. 41, 1161-1172.

Keywords: teaching of crystallography, training, X-ray crystallography of biological macromolecules

# MS46-T04

Applications of the Cambridge Structural Database in Chemical Education. <u>Gary M. Battle</u>. *Cambridge Crystallographic Data Centre*, 12 Union Road, *Cambridge*, UK. E-mail: <u>battle@ccdc.cam.ac.uk</u>

The Cambridge Structural Database (CSD) represents a vast and ever growing compendium of accurate 3D structures that has massive chemical diversity across organic and metalorganic compounds. For these reasons, the CSD is finding increasing application in chemical education. This talk will introduce a teaching subset of more than 500