CCP4/APS School in Macromolecular Crystallography: From data collection to structure refinement and beyond

The CCP4/APS School in Macromolecular Crystallography was held at the Advanced Photon Source (APS) synchrotron site at Argonne National Laboratory, near Chicago June 7th to June 15th 2011. This was the fourth time the school was organized. It was organized by the APS beamlines 23ID-B and 23ID-D of the General Medicine and Cancer Institute Collaborative Access Team (GM/CA-CAT) at APS and Collaborative Computational Project No. 4 Software for Macromolecular X-Ray Crystallography. 20 graduate students and postdoctoral researchers in the area of structural biology from all over the world were selected to attended the school. The workshop covered all aspects of the structure solution process in macromolecular crystallography, starting from data processing, through phasing and refinement, and ending with validation and deposition.

The two first days were assigned to data collection and all students were encouraged to bring their own crystals for data collection. While collecting data, experts were discussing which data collection strategy would be best for which type of crystal with the students. The following days covered the areas of processing the diffraction data, phasing, refinement and validation. The outline of the program was following: lectures about the theoretical background of software packages in the morning, tutorials on the software packages discussed in the afternoon sessions and in the evening sessions the students worked on their own data, either diffraction data collected at site or some data set brought to the school. The evening sessions also functioned as problem solving sessions as the students had brought especially difficult data sets.

The workshop covered many of the programs used for data processing and structure solution. Some of the programs covered were; Mosflm, Scala, HKL2000, XDS, Refmac, ArpWarp, PHENIX, Phaser, Coot, SHELXC/D/E, Balbes, Mrbump and Buccaneer. I enjoyed the school a lot and I can recommend it to any student working in the field of structural biology. However, some knowledge of data processing and refinement is preferred as the course is rather intense and advanced. I especially enjoyed and appreciate the personal feedback and advices the program developers gave during the problem solving sessions when we worked on our own data. The program for the course was very well planned with theoretical lessons, tutorials and problem solving sessions.

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