

increase enzymatic activity. The structure suggests that interaction with the membrane is mediated by one of the p85 domains (iSH2). The existence of p110alpha gain-of-function-mutants makes this protein an attractive therapeutic target. Since PI3Ks control a wide range of physiological functions, it would be desirable to inhibit only p110alpha, the isoform mutated in cancers. Structural differences among the isoforms can be exploited for that purpose. These findings may provide not only novel insight for the design of PI3K-isoform-selective drugs but also help on the design of mutation-specific drugs.

Keywords: PI3K, p110alpha, drug design

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Is there a steep learning curve in crystallography?

Michael Ruf, Joerg Kaercher

Bruker AXS Inc., 5465 East Cheryl Pkwy, Madison, WI, 53711, USA, E-mail: michael.ruf@bruker-axs.com

The synthesis of aspirin is a part of many undergraduate organic classes. These courses teach synthesis skills and introduce students to purification using re-crystallization. Typically good quality crystals for single crystal x-ray investigation can be obtained within a few hours from the start of the experiment. As crystallography provides the most unambiguous structural information of all analytical tools it seems a natural progression to introduce students to this technique at an early stage and not reserve these tools for cutting edge research. Advances in chemical crystallography have traditionally focused on improving individual components of instrumentation and software algorithms. The next quantum leap is the development of fully integrated configurations, where several crystallographic methods are combined on a single accelerator platform. This allows for the full streamlining of the traditionally tedious and time consuming process of determining the three dimensional structures of molecular compounds. This talk tries to look critically at new, easy, and intuitive x-ray crystallographic methods for 3-D structural characterization. It questions whether user-friendly automated system operation generates reliable data without extensive crystallographic knowledge and can overcome the steep learning curve in crystallography.

Keywords: software automation, hardware automation, teaching

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A tutorial for learning and teaching macromolecular crystallography

Annette Faust¹, Santosh Panjkar¹, Uwe Mueller², Venkataraman Parthasarathy¹, Andrea Schmidt¹, Victor S Lamzin¹, Manfred S Weiss¹

¹EMBL, ²BESSY GmbH, BESSY-MX group, Albert-Einstein-Str. 15, D-12489 Berlin, Germany, E-mail: Faust.Annette@embl-hamburg.de

Based on five diffraction data sets collected during the DGK(german crystallographic association)-workshop on X-Ray Diffraction Data Collection using Synchrotron Radiation held at the BESSY synchrotron (Berlin, Germany), we have assembled a tutorial for teaching and learning macromolecular crystallography with the emphasis on crystallization, diffraction data collection and processing, and automated structure solution. The tutorial consists of five experiments. It covers all the information needed to repeat

the whole experiments or parts of it starting from the crystallization and ending with the structure determination. The material provided includes also the raw X-ray data. The five experiments are (1) structure determination by sulphur-SAD (single wavelength anomalous diffraction) on cubic insulin, (2) structure determination by MAD (multiple wavelength anomalous diffraction) on bromide-soaked thaumatin, (3) structure determination by molecular replacement on monoclinic hen egg-white lysozyme, (4) the identification of bound surface ions and (5) the identification of an active site ligand in tetragonal lysozyme crystals. For the later two projects, the diffraction data were collected using longer X-ray wavelengths. The tutorial and/or the provided X-ray data can be used in hands-on workshops in macromolecular crystallography or as material for lectures. The material can also help beginners in the field of macromolecular crystallography to gain first experience in crystallization, data collection and the use of crystallographic software to determine three-dimensional macromolecular molecule structures. Detailed description of the five experiments and all available material including the raw X-ray data will be made available for download from the authors' webpages.

Keywords: crystallographic teaching, X-ray diffraction of macromolecules, three-dimensional protein structure

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The web-based teaching in the Institute of Structural and Molecular Biology, University of London

Snezana Djordjevic¹, Tracey Barrett^{1,2}, Jim Pitts^{1,2}, Christine Slingsby^{1,2}, David Moss^{1,2}, Clare Sansom^{1,2}, Nicholas Keep^{1,2}

¹University College London, Institute of Structural & Molecular Biology, Darwin Building, Gower Street, London, England, WC1E 6BT, UK, ²School of Crystallography, Birkbeck, University of London, E-mail: snezana@biochem.ucl.ac.uk

Birkbeck, University of London initiated the teaching of structural biology over the web in 1995, with the inaugural Principles of Protein Structure Course. This course can now be combined with a further web based modules in Protein Crystallography or Techniques in Structural Molecular Biology and project work to form the MSc in Structural Molecular Biology <http://www.cryst.bbk.ac.uk/mscstructuralbiology.html>. Students study blocks of course material released as password protected web pages. They interact with the module tutors via email/chat rooms and coursework is submitted electronically either via web forms or email. Written exams can be sat in universities or British Council offices around the world bypassing the need to travel to Birkbeck. The Commonwealth Scholarship Commission has awarded us scholarships for students based in developing Commonwealth nations, and internet bandwidth is still very much a consideration for these students. Nevertheless improved computer performance over the last 12 years has made delivery of the course easier. This is illustrated by the fact that in the early years, students would upload program scripts to servers at Birkbeck in order to perform crystallographic calculations, but can now run CCP4 software on their own machines. Similarly, Jmol images embedded in web pages have largely replaced downloading RasMol scripts.

Keywords: teaching aids, world wide web, teaching of crystallography