Crystallography Times

Protein Crystallography Newsletter
Volume 2, No. 2, February 2010

In this issue:

Continuing Education Webinar
Practical Approaches to Data Processing Using XDS
Presenter: Dr. Kay Diederichs
February 25th at 9AM EST
(14:00 GMT)

Kay Diederichs will provide an overview of X-ray diffraction image processing with XDS. Kay created the XDSwiki in 2008 to provide an accurate and up-to-date resource for XDS users. He contributes to the development of XDS and is the author of XDSSTAT, a program that provides additional analytical tools for XDS output. Kay is also the originator of the CCP4wiki and a frequent contributor to the CCP4bb. He is currently a Professor at Universität Konstanz.

Spring Webinar Series Focuses on Software

Note that our continuing webinar program will feature well known expert presenters in a mini-series devoted to commonly used data processing packages.

Rigaku Alchemist II

Crystallography in the news

February 17, 2010. University of Alabama in Huntsville crystallographer and Associate Professor Joseph D. Ng witnessed and commented on the faculty meeting shooting spree that left three faculty members dead and three others wounded within the Department of Biological Sciences.

February 16, 2010. University of Missouri researchers, led by John Tanner, were able to visualize the donut-shaped structure of an enzyme that degrades proline, which is an amino acid that has a central role in metabolism.

February 13, 2010. Academia Sinica Vice President Andrew H.-J. Wang and his team from the Institute of Biological Chemistry (IBC) used x-ray crystallography to solve the structure of an enzyme involved in the production of the scent given off by the mint plant.

February 12, 2010. The Oklahoma Medical Research Foundation, led by Stephen Prescott, has entered into a strategic partnership with one of China's premier research facilities, the Institute of Biophysics, Academy of Chinese Sciences in Beijing. This collaboration will allow the institutions to share researchers and equipment in the field of structural biology.

January 24, 2009. The complete atomic-level architecture of a brain protein critical to movement, memory, and learning - called a glutamate receptor - caps more than 11 years of painstaking work by a team of scientists led by Eric Gouaux of the Oregon Health and Science University.

Custom screens without pumps and tubing

Traditional methods of creating crystallization screens can be complex and time consuming as well as inherently limited by potential issues of contamination, human error, and dispense accuracy. The Rigaku Alchemist™ II screen making system addresses these issues with its revolutionary patented BirdFeeder™ technology. This unique self-contained liquid dispensing and storage device allows for individual stock solution management, with barcode tracking, individual syringes to assure no cross contamination, and integral long-term storage, all in one easy design. Eliminating clogged lines and valves, Alchemist II can dispense screens directly in to either deep well blocks or into VDX/Linbro/Nextal plate formats.

Alchemist II is completely self-contained: no external water, no external waste. Instead of tubes, pumps and pipettes, the Alchemist II uses 1 container (BirdFeeder) and 1 syringe per solution. A different BirdFeeder and syringe is used for each different solution. So *cross-contamination is not possible*. Since there is no pre or post-experiment rinsing needed, the setup of an experiment is FASTER than instruments that utilize tubes. BirdFeeder IDs and locations on the deck of the Alchemist II are managed via barcodes. The small size of the BirdFeeders allows for 72 BirdFeeders to be set up on the deck at once. Consequently, all 66 solutions needed to make a Hampton Screen HT can be set up on the deck of the Alchemist II at once.

Request more information on Alchemist II.

Lab spotlight: ESFRI-INSTRUCT - Core Center G

Within the Department of Molecular Membrane Biology at the Max-Planck-Institut für Biophysik in Frankfurt resides the ESFRI-INSTRUCT - Core Center G.

Rigaku Alchemist II screen maker (top). Exploded diagram of a BirdFeeder assembly illustrating the integration of a dedicated syringe with a stock solution reservoir.

Dr. Yvonne Thielmann and Dr. Juergen Koepke pictured (top) in from of the Minstrel™ HT and Gallery™ 700 modules of their new Rigaku CrystalMation™ system at the ESFRI-INSTRUCT - Core Center G facility in Frankfurt, Germany.

The bottom image is from the recent open house for the CrystalMation system in Europe, which was attended by over 100 guests consisting of local, state and UE government officials as well as Max-Planck Institute executives. At the event, Dr. Yvonne Thielmann gave a lecture on CrystalMation system and how this will help advance research.

Upgrading and expanding the X-ray crystallography facility at the Max-Planck Institute of Biophysics was part of a recent initiative by ESFRI-INSTRUCT (European Strategy Forum on Research Infrastructures - Integrated Structural Biology Infrastructure) to elevate the Max-Planck Institute of Biophysics to be one of the seven core European centers for structural biology.

Prof. Dr. Dr. h.c. Hartmut Michel, winner of Nobel Prize for Chemistry in 1988, leads the Department of Molecular Membrane Biology which oversees Core Center G. For the preparatory phase, the BMBF (German Ministry of Education and Research) has funded the effort, with the majority of the funds being invested to improve the X-ray crystallographic equipment managed by Dr. Juergen Koepke. The center now includes two Rigaku rotating anode based crystallography systems (MicroMax™-007 HF and a FR-E+ SuperBright™ X-ray sources) and a CrystalMation automated crystallization system tended by Dr. Yvonne Thielmann.

Useful links for crystallography

DaRa server is a DAtabase for RApid search of structural neighbors for proteins based on their X-ray small-angle scattering patterns. To optimize the search, the experimental data has to be first processed by the program GNOM. DaRa directly reads in the output file given by GNOM, and you only need to specify the molecular mass of the protein to define the section of the database to be screened.

Folding@home is a distributed computing project, run by Pande lab at Stanford University, where people from throughout the world download and run software to band together to make a virtual supercomputers dedicated to understanding protein folding, misfolding, and related diseases.

Selected recent crystallographic papers

Structural basis for dsRNA recognition and interferon antagonism by Ebola VP35. D.W. Leung, K.C. Prins, D.M. Borek, M. Farahbakhsh, J.M. Tufariello, P. Ramanan, J.C. Nix, L.A. Helgeson, Z. Otwinowski, R.B. Honzatko, C.F. Basler and G.K. Amarasinghe. *Nature Structural & Molecular Biology* **17**, 165-172 (2010).

Alda-1 is an agonist and chemical chaperone for the common human aldehyde dehydrogenase 2 variant. S. Perez-Miller, H. Younus, R. Vanam, C.H. Chen, D. Mochly-Rosen and T.D. Hurley. *Nature Structural & Molecular Biology* **17**, 159-164 (2010).

Coupled chaperone action in folding and assembly of hexadecameric Rubisco. C. Liu, A.L. Young, A. Starling-Windhof, A. Bracher, S. Saschenbrecker, B.V. Rao, K.V. Rao, O. Berninghausen, T. Mielke, F.U. Hartl, R. Beckmann and M. Hayer-Hartl. *Nature* **463**, 197-202 (2010).

Helicobacter pylori CagA inhibits PAR1-MARK family kinases mimicking host substrates. D. Nesic, M.C. Miller, Z.T. Quinkert, M. Stein, B.T. Chait and C.E. Stebbins. *Nature Structural & Molecular Biology* **17**, 130-132 (2010).

Structural analysis of an MK2-inhibitor complex: insight into the regulation of the secondary structure of the Gly-rich loop by TEI-I01800. A. Fujino, K. Fukushima, N. Namiki, T. Kosugi and M. Takimoto-Kamimura. *Acta Crystallographica Section D* **66**, 80-87 (2010).

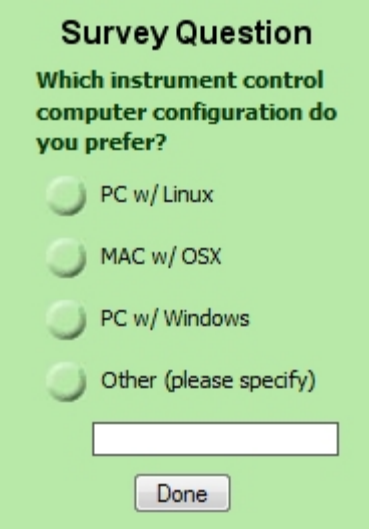
Structure of a family 3b' carbohydrate-binding module from the Cel9V glycoside hydrolase from *Clostridium thermocellum*: structural diversity and implications for carbohydrate binding. S. Petkun, S. Jindou, L. J. W. Shimon, S. Rosenheck, E. A. Bayer, R. Lamed and F. Frolow. *Acta Crystallographica Section D* **66**, 33-43 (2010).

Book review: *The Structure of Scientific Revolutions*

Rigaku Hardware Training Classes

Rigaku will hold two training sessions, at our Texas facility, tailored towards the needs of macromolecular crystallographers and their staff. Course format will be a series of short lectures on theory followed by hands-on activities with detectors and X-ray generators. Safety will be emphasized. Click for more info on upcoming sessions:

- March 24-26, 2010
- October 27-29, 2010



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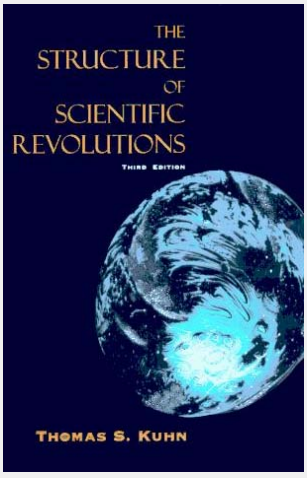
into your browser.



by Thomas S. Kuhn

I came across references to this book in reading three other books at the end of last year. I thought to myself that I should read it, and I have, twice. The first scientific book I started reading this year mentioned TSoSR. I am reaching the conclusion that I must be the only person who hadn't read it.

The main concepts described include the terms "paradigm", "normal science" and "revolutionary science." Kuhn describes a paradigm as being the prevailing model or theory describing a phenomenon. Normal science is the process by which incremental improvements add to the existing paradigm. Kuhn suggests that most science is normal - which a point of contention for many. Revolutionary science is the result of a crisis or crises in which the extant paradigm no longer describes the observations. Kuhn does stress the observer's frame of mind is important, as two observers may see the same picture yet interpret it completely differently. When revolutionary science works, a paradigm shift occurs. Kuhn also suggests that those creating the paradigm shift may not be aware of the shift, and that the actual revolution may only be observable from a historical perspective.

Kuhn also spends time discussing the concept of incommensurability (not related to lattices at all). This idea is used to describe a new paradigm that is essentially orthogonal to the old paradigm ... where the descriptors of the old fail to work with the new, and communication between scientists fails. Obviously, this creates a problem in the transition from old to new.

Kuhn first this published this philosophy book in 1961. A third final edition was published in 1996, the year Kuhn died. This book has been referred to as one of the hundred most influential books since World War II by the *The Literary Times* and the best exposition of the scientific method by the *New York Times*. Is it? You'll have to decide for yourself.

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